This is to certify that the

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Adiabatic Propagation of Phase Boundaries
in a Thermoelastic Bar

presented by

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has been accepted towards fulfillment
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Major professor

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ADIABATIC PROPAGATION OF PHASE BOUNDARIES IN A THERMOELASTIC BAR

By

Ralph Worthington

A DISSERTATION

Submitted to
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ABSTRACT

ADIABATIC PROPAGATION OF PHASE BOUNDARIES IN A THERMOELASTIC BAR

By

Ralph Worthington

A Helmholtz free energy function is introduced for a one dimensional two phase solid. The free energy accounts for both thermal and mechanical effects. Phase transformations can occur between two distinct phases, one in which the stress response is dependent on the both the deformation and current temperature, while the other is independent of any thermal effects. The model admits a thermomechanical coupling parameter α_2 which can be associated with a coefficient of thermal expansion in the thermomechanical phase. If the coupling parameter α_2 is set to zero, then one retrieves results from what is known as the separable theory.

A set of initial conditions are proposed such that a single phase boundary is present in a stable equilibrium configuration. Such configurations are shown to be a two parameter family of states. The initial configuration is disturbed by a set of dynamic boundary conditions that give rise to a wave pulse, the wave propagates from one of the boundaries into the interior of the bar. This travelling wave eventually encounters and interacts with the phase boundary, and it is shown that the encounter is characterized by a one parameter family of solutions. The fully thermomechanical theory is treated analytically in the small α_2 limit, and thermal effects are shown to play a major role in the interaction. The Clausius-Duhem inequality is shown to restrict the family of solutions.

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Professor David Yen

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1. Introduction

1.1 Overview

Recently, the topic of solids able to undergo phase transitions has received a great deal of attention from the mechanics community. In this section we will briefly introduce topics pertaining to phase transformations in order to familiarize the reader with the research to be presented. It is well known that certain materials which behave elastically can be modeled with a stress-strain response derivable from a potential function. Classically this potential function is defined as the material's strain energy density and is usually a convex function, resulting in the equilibrium equations being elliptic in nature. Typically this gives rise to a stress-strain response which is one to one, i.e. associated with each stress there exists a unique strain. However, if the materials potential function is not convex, then the equilibrium equations may lose ellipticity. This may result in the stress-strain response losing the one to one behavior, and for certain levels of stress the associated strains may not be unique. It is this non-determinacy which makes these problems both mathematically challenging and representative of phase transformation phenomena.

Figure 1.1 is a schematic diagram of a hypothetical material in which the strain energy density W is not a convex function of some strain component γ, say tensile strain. If one were to consider a tensile test of a specimen composed of such a material, with a load being applied to the specimen resulting in the stress being contained in the range $\sigma_m \le \sigma(\gamma) \le \sigma_M$, then it is seen from this figure that the material need not be in a state of homogeneous deformation. It may be that the specimen contains regions of strain that differ radically, some regions being in a state of "low" strain adjacent to one in a different state

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state of "high" strain. Thus, the possibility exists that within the body there exist surfaces that separate regions of low strain from high strain, and across such surfaces the strain suffers a discontinuity. These surfaces are called phase boundaries, while the material itself on either side is said to occupy a particular phase. A region of a material undergoes a phase transition when it transforms from one phase into another.

For materials capable of undergoing these types of transitions the study of equilibrium configurations, quasi-static and dynamic motions is possible. In all three areas, the ability of the body to transform between different phases and generate phase boundaries is of interest. For quasi-static and dynamic problems one must consider the possibility of a moving phase boundary, and the interaction of such a boundary with other surfaces.

Further complicating the issue is the addition of temperature effects. In general, research into the purely mechanical motions of such materials has received more attention then the modeling of thermal motions. The latter, however, is now also becoming an area of increasing research activity.

1.2 Literature Review

In general a material can be thought of undergoing a phase transition when properties that characterize the material change in response to a state variable reaching a critical value. Examples of such transitions are between liquid and gas, solid and liquid, as well as solid to solid and other combinations. The model for the van der Waals fluid captures such behavior, where at constant temperature it is either a fluid or vapor depending the level of its specific volume. In the case of solids, the generic ausenite/martensite transition comes to r

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to mind, where depending on the level of temperature and stress the solid may be in either state, the states having different material properties. Furthermore this type of solid to solid transition is the mechanism for the shape memory effect. In what is to follow we will discuss an elastic solid in which the stress strain response is not monotone, and allows for discontinuous field quantities which may be interpreted as a solid undergoing a phase transformation.

The study of elastic solids experiencing discontinuous field variables has received a great deal of attention in previous decades and the literature concerning this topic is now quite extensive. From a mechanistic point of view, one may think of three different classes of problems: equilibrium, quasi-static, and the fully dynamical problems. Some of the more relevant literature which addresses these types of problems will be explored below.

In (1975), Ericksen discussed an elastic bar in equilibrium having a non-monotonic stress-strain relation. For a range of stresses and displacements this type of response allows for more than one strain to be realized. When the bar is subjected to the boundary conditions of a controlled load or displacement (soft or hard device) it is shown that infinitely many equilibrium configurations are possible. In an attempt to rectify this deficiency, the author studies an energy minimization criterion in a attempt to determine a unique and stable solution. Thus he demonstrated that for certain nonlinear elastic materials, a bar composed of such a material subjected to specific load/displacement boundary data may not support an unique solution. The author states that one may interpret this ability of the solid elastic material to accommodate a range of strain for the associated specified stress as a solid undergoing a solid to solid transformation. This ability to model a phase transformation in a solid via the nonmonotone stress-strain response has greatly cont

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contributed to research efforts in this phenomena.

Knowles and Sternberg (1978), in the setting of plane non-linear elastostatics, demonstrate that a certain set of deformations having continuous displacements posses the property that the displacement gradients may be discontinuous In elastostatics, the equations of equilibrium which govern the deformation fields are classified as elliptic partial differential equations, and when discontinuities in the deformation gradients arise, the classification of these governing equations changes from elliptic to hyperbolic; the equations are said to lose their ellipticity. Thus within a hyperelastic solid one can construct solutions such that the displacement field is everywhere continuous, yet the deformation gradients may be piecewise continuous as long as the equilibrium equations suffer a loss of ellipticity. Therefore surfaces may exist such that the deformation gradients suffer a jump in value when passing from one side of the surface to the other, and these jumps in field quantities may be attributed to the material undergoing a phase transformation. The authors refer to such a singular surfaces as an "equilibrium shock", however now the term phase boundary is more widely used. The existence of such a discontinuous surface leads to an additional system of equations which connect the field quantities adjacent to the surface, these equations are the Rankine-Huginot equations.

If one considers a body capable of containing these types of discontinuities, then families of equilibrium states parameterized by time may be constructed so as to yield the quasi-static evolution of a phase boundary. During such quasi-static motions the total energy may change, thus the passage of a phase boundary may dissipate the energy within the body. Knowles and Sternberg explore the quasi-static evolution of a phase boundary through an elastic body and the dissipation of energy which occurs during such processes.

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They demonstrate that the equations which govern such processes are similar in form to those of steady irrotational flows in a compressible inviscid fluid.

The dissipation of energy during the motion of a phase boundary directs one to inquire as to the use of certain evolution criteria during these types of motions. For quasi-static motions Knowles (1979) investigates the dissipation of energy, and from the second law of thermodynamics derives a dissipation inequality for a three dimensional body. He demonstrates for all motions of a phase boundary that the dissipation should be nonnegative. A dissipation function is derived and shown to be a function of the energy momentum tensor, also known as the driving traction or force on the defect, whose effects in a different context where previously studied by Eshelby (1975).

For such quasi-static evolution problems, the lack of uniqueness of a solution is found to be even more extreme than the equilibrium problem. The reason being that each equilibrium configuration is indeterminate for the reasons outlined above, and the speed of the phase boundary through the material inherits this indeterminacy. Various procedures have been proposed to resolve this issue of determining a unique solution among the infinite number of admissible candidates. One type of selection criterion is to impose an energy minimization condition to each equilibrium configuration during the evolution of a phase boundary. This results in the driving traction being equal to zero for each equilibrium state. Another approach requires all motions to occur with maximum dissipation of energy. Instead of using an energy platform, one may introduce an additional set of constitutive relations, a nucleation criterion and kinetic relation. The former imposes conditions on the emergence of phase boundary, while the later governs the actual evolution of the boundary. Abeyaratne and Knowles (1988) use this method to resolve the issue of nonuniquer

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niqueness for a one-dimensional, isothermal, elastic bar whose stress strain response is non-linear.

In the fully dynamical motion of a phase boundary, the governing equations are different from the quasi-static case due to the additional inertia terms. Within the dynamics of elastic bars, James (1980) studies some general properties of solids containing propagating phase boundaries. Abeyaratne and Knowles (1990a), investigate the Riemann problem of a bar which has a non-monotonic, tri-linear stress strain response. They show that the lack of a unique solution can be rectified by the use of a kinetic relation and a nucleation criterion, as for the quasistatic case. With these two additional criteria the authors study the solution for the propagation and interactions of phase boundaries within the bar.

For a body consisting of a elastic layer of finite thickness Pence (1991a) investigates the initial interaction of a incoming shear pulse with a single stationary phase boundary and the subsequent ringing of shear waves between the external boundaries and the internal phase boundary. The author specifies that a single phase boundary is initially present, and pursues a treatment that excludes additional phase boundary nucleations. He then proceeds to investigate the family of solutions parameterized by the phase boundary speed. Various impedance criteria are used as a selection technique for the phase boundary speed. It is shown for the special case of a completely reflecting or transmitting wave interaction with the phase boundary, that the motion of the phase boundary is periodic in nature. In another study, Pence (1991b) examines the same problem from the perspective of energy and dissipation. Using a criterion based on the dissipation within the layer, it is shown that there are exactly two motions which permit no dissipation, and one motion that maxin

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maximizes the dissipation rate. In Abeyaratne and Knowles (1992a), (1992b) a set of similar problems of the interaction of a wave pulse and a stationary boundary are treated.

Another approach for resolving the issue of nonuniqueness is to attribute structure to the phase boundary, essentially giving it a finite thickness and matching conditions within the boundary to the conditions at the interface. Slemrod (1983) uses this approach for isothermal motions of a van der Waals fluid. Although the material model is nominally for a fluid, the equations which govern the processes are mathematically similar to those of a solid and thus the associated ideas apply to solid-solid modeling. The reader interested in all the above techniques should see Truskinovsky's (1991) paper which comprehensively discusses the formulation and results using these methods for a broad class of problems.

So far all of the above papers cited concerned motions, whether quasi-static or dynamic, which were assumed to proceed isothermally. The literature for motions which occur without the isothermal constraint is more limited. James (1983) considers the steady propagation of a phase boundary within a thermoelastic bar, allowing for changes in temperature during a dynamical process. Under the assumption that all motions within the bar are close to an equilibrium state, he is able to show for adiabatic motions that the governing equations are unable to determine a unique solution, and thus the addition of thermal effects does not resolve the issue of uniqueness.Truskinovsky (1985) is one of the first to investigate thermal effects for motions within a heat conducting nonlinear elastic bar. He resolves the issue of nonuniqueness by attributing structure to the phase boundary. Gurtin (1991) explicitly formulates the general laws which govern all motions for the thermomechanical propagation of a phase boundary. In Abeyaratne and Knowles (1993a) a stress-strain

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strain-temperature response function is introduced for a material able to undergo phase transitions. This response function is piecewise continuous for the different phases of the material. From the appropriate stress response function the free energy density is constructed for either phase using thermodynamic arguments. They introduce a kinetic relation and then study the hysteretic response of the material for quasi-static motions.

The Clausius-Duhem inequality is a thermodynamic restriction on all admissible motions for the above mentioned problems. It can be used to eliminate possible candidates for solutions produced from the other field equations, but it will not provide a unique solution. This inequality may be reformulated by the construction of an entropy production function for processes occurring within a body, and for all admissible motions the entropy production must be nonnegative. Abeyaratne and Knowles (1990b) show for a three dimensional body with a continuous temperature field that the rate of entropy production occurring during the motion of a phase boundary consists of three parts: one from the material dissipation away from phase boundary, a second part which arises from heat conduction, and a contribution from the moving phase boundary. Restricting the class of materials to that which is thermoelastic they show that the rate of entropy production is due only to heat conduction and the motion of the phase boundary.

Mathematically, the above equilibrium problems give rise to a system of elliptic partial differential equations (PDE). When these equations admit solutions which have continuous displacements, but displacement gradients which are discontinuous, then the form of these equations changes from elliptic to hyperbolic. In the case of fully dynamic phase boundary motion one has the additional inertia terms and the classification of the governing equations is now normally hyperbolic. With respect to engineering applications and applied mathematics, hyperbolic PDE's were studied extensively in the context of gas dynamics, see Courant and Friedrichs (1956) or Landau and Lifshitz (1987).

The class of boundary value problems presented in this document are typically found in the studies of systems of hyperbolic equations. Lax (1973) considers a very general form for systems of hyperbolic PDE's or conservation laws, and displays certain aspects of their nature and also addresses the admissability criteria for weak solutions of such systems. Hattori (1986) considers the Van der Waals fluid, governed by a specific system of conservation laws, for which he proposes a maximum entropy rate admissability criterion for all solutions. Truskinovsky (1991) also works with discontinuous solutions which occur in these types of systems, and explores the implications of various physical models which may be taken as a basis for the conservation laws.

Thermodynamically, a phase transformation is classified according to the type of discontinuity present in the materials free energy (Rao and Rao 1978). A first order phase transformation is characterized by a material free energy that is continuous, but whose first derivatives are not. A second order transformation is similarly described by a continuous first derivative, but a discontinuous second derivative. One may also speak of mixed order transformations. However in this document the problems considered will be exclusively first order.

Various authors have proposed models for the material in which the materials free energy possesses the required continuity, and yet still allows for transitions to occur. Falk (1980) proposes a function for a Helmholtz free energy to model the phase transition between Austenite/Martensite. The function is of the Landau-Devonshire type and is capable of supporting first order transitions. The author derives the fundamental properties of suc

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such a material, and discusses the phenomena of shape memory and hysteresis which the model allows. Niezgodka and Sprekels (1988) derive the necessary equations which govern a thermomechanical dynamical phase transition. Introducing a Landau-Devonshire model for the material's free energy into the governing equations results in a system of coupled non-linear partial differential equations.

The free energy function introduced in this document will not be of the Landau-Devonshire type. Since we wish to focus our attention on that subset of the material's response for which a transformation can take place, and not the entire spectrum, we utilize an efficient method of constructing a material model. By constructing a free energy function composed of a set of discrete functions, one for each phase, and requiring the continuity of this function at transition points, the model is able to capture first order phase transitions. This discreteness allows us to use a lower order polynomial for the free energy, which in turn simplifies the mathematics.

1.3 Problem Statement

The material within this document can be thought of as being composed of two major parts. The first part consists of Chapters 1-4, the second consists of Chapters 5-9. We begin by first introducing the field equations for a one dimensional continuum, we consider a bar, where the equations are specialized to account for adiabatic motions only. Since we wish to consider the motion of phase boundaries, the Rankine-Hugoniot equations are presented. These being jump conditions for the field variables between regions separated by a discontinuitys surface. Here this surface is initially motionless and so constitu

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stitutes an equilibrium phase boundary. Eventually it is set in motion via the introduction of a wave pulse.

In Chapter 3 we develop a 1-D constitutive model for a solid able to undergo phase transformations. A model for the Helmholtz free energy model is developed, it is a function of the strain and temperature, and can be thought of as a "potential well". The free energy is constructed in such a manner so as to accommodate two distinct phases. One of the major differences between the two phases is that only one possesses a shape strain. The stress response is derived from the free energy, one phase has a stress response that is independent of temperature while the other is temperature dependent. From it's two phase nature, the stress-strain curve is nonmonotonic. One feature of the nonmonotonic behavior is the lack of uniqueness involved in a equilibrium configuration, even by specifying the temperature and stress, or temperature and elongation, the state of strain within the bar is not unique. We show that the equations of equilibrium characterize a two parameter family of configurations.

In Chapter 4 we investigate this lack of uniqueness in equilibrium configurations in detail. There we introduce three canonical equilibrium configurations, each configuration having a separate criterion in addition to the equations of equilibrium.These canonical states are families of one parameter equilibrium configurations. We then demonstrate that when any two of the three states coincide, then the resulting equilibrium configuration is a unique state. These unique equilibrium states play a central role in understanding the connection between the present fully thermomechanical description, and simpler descriptions that are purely mechanical in nature

To begin the second part of this document we formulate and impose a set of initial

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conditions such that a single phase boundary is present in an equilibrium configuration. This initial configuration is then disturbed by a set of dynamic boundary conditions which give rise to a wave pulse that propagates into the bar from one of the boundaries. This travelling wave eventually encounters and interacts with the phase boundary, it is this interaction that we later investigate in detail. In general, this interaction causes the phase boundary to move, leading to phase transformations as particles pass through the moving phase boundary.

A temperature-independent version of this problem was considered by Pence (1991a, 1991b). In his work a layer was composed of a two phase elastic material, but the stress response was independent of thermal effects in both phases. The mathematical equations which compose Pence's problem are identical to ours. In Chapter 5 we modify this purely mechanical problem so that we may compare any solutions from our problem with those from the purely mechanical problem. One of the major goals of this research is to extend this previous work so as to encompass thermal effects, and demonstrate any new features of our more complete physical theory.

The interaction of the incoming wave pulse with the phase boundary gives rise to two possible scenarios regarding the transmitted wave that becomes the leading disturbance after the interaction. The first involves a shock, the other involves a centered simple wave fan. We only consider the latter case in this document. In Chapters 6 and 7 we develop a system of algebraic equations which completely characterizes the initial interaction. This system of equations is indeterminate, there being more unknown field quantities than equations. Considering the phase boundary speed as a parameter, we are able to reduce the system of equations to a singe master equation, a nonlinear algebraic equation for

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for a single field variable. A solution to this equation not being evident, we develop a solution, albeit a family of solutions, for the unknown field variable via a perturbation from the purely mechanical state. We show once this perturbation solution is constructed that we can than calculate all the remaining field quantities. By comparing our results with those from the purely mechanical problem we are able to determine the leading order thermal effects, which is one of the major objectives of this research.

In Chapters 8 and 9 we demonstrate how the second law of thermodynamics restricts this family of solutions. Finally, we consider an additional constitutive relation, a kinetic relation between the phase boundary speed and the driving traction acting on the phase boundary. We show that this additional criterion singles out a unique solution to the interaction.

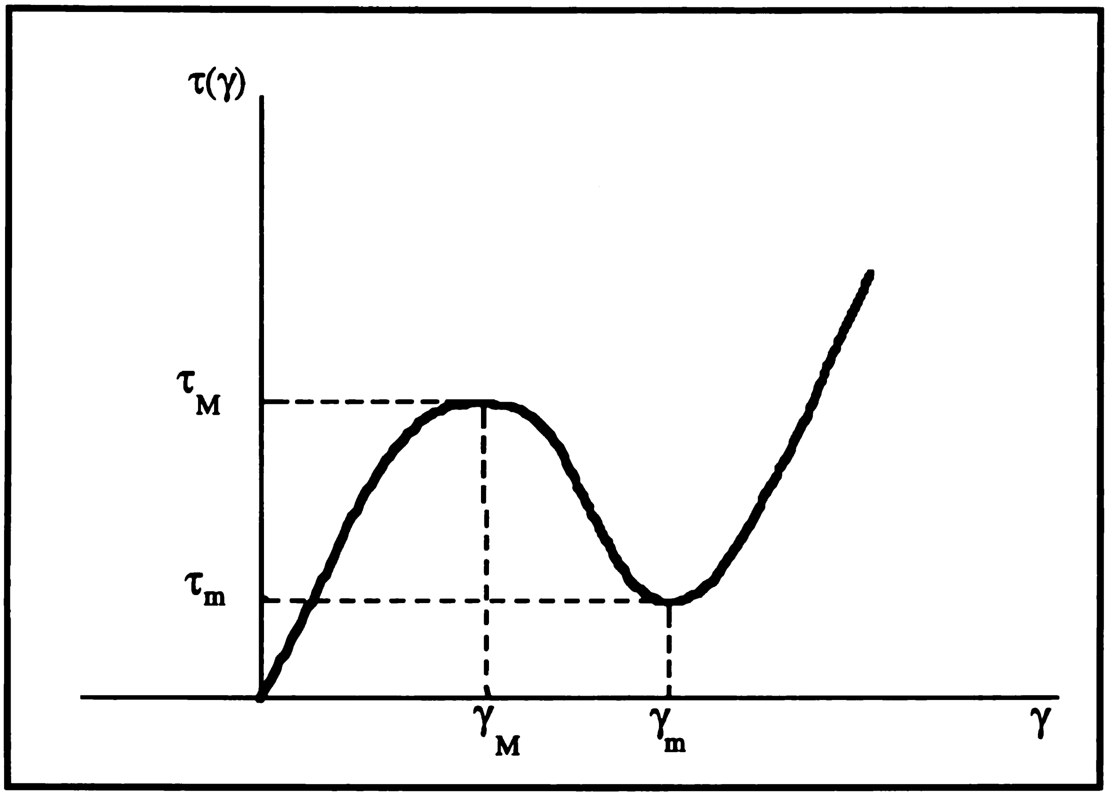

Figure 1.1 Displayed is the nonmonotonic stress strain response for the material model describing phase transformations. Note for the prescribed level of stress in $\tau_m \leq \tau \leq \tau_M$ that there are three possible values for the strain γ

2. Balance Laws

Consider a body $\mathcal{B}$ which is a bar of length L and of constant unit cross section. Let $\underset{\sim}{e}_i$ denote the triad of mutually orthogonal unit vectors associated with the reference configuration, where $\underset{\sim}{e}_1$ is parallel to the rod's axial direction. Denote the position vector of a particle in the reference configuration by $\mathbf{x}$, then

$$\mathcal{B} = \{ (x_1, x_2, x_3) \| x_1 \in [0, L] \}.$$

Let the position of the particle $\mathbf{x}$ at time t be $\mathbf{y}(\mathbf{x}, t)$, the deformation of the bar, and consider motions of the type:

$$\mathbf{y}(\mathbf{x}, t) = \mathbf{x} + u(x_1, t)\underset{\sim}{e}_1, \tag{2.1}$$

where the function $u(x_1, t)$ is the displacement of the particle. Deformations of the form (2.1) describe longitudinal deformations of the bar. The problem is essentially one dimensional, therefore let $x_1 = x$ for notational convenience.

In what is to follow the displacement $u(x_1, t)$ is assumed to be a continuous function almost everywhere with first and second derivatives which are piecewise continuous. Denote the strain in the bar as γ and the velocity v, then by definition

$$\gamma = \frac{\partial u}{\partial x}, \tag{2.2}$$

$$v = \frac{\partial u}{\partial t}. \tag{2.3}$$

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The strain γ is required to satisfy $\gamma > -1$ in order for the deformation (2.1) to be invertible.

Introduce the following notation, let

τ denote the stress,

ε the internal energy per unit volume,

η the entropy per unit volume,

q the heat flux,

θ the absolute temperature,

r the heat supply per unit mass, and

ρ the mass density.

Using a Lagrangian description, the local equations of motion (Dunn and Fosdick 1988) for the bar are:

$$\begin{aligned}
\frac{\partial \gamma}{\partial t} &= \frac{\partial v}{\partial x}, \\
\rho\frac{\partial v}{\partial t} &= \frac{\partial \tau}{\partial x}, \\
\frac{d\varepsilon}{dt} &= \tau\frac{\partial v}{\partial x} + \rho r - \frac{\partial q}{\partial x}, \\
\frac{d\eta}{dt} &\geq \frac{r}{\theta} - \frac{1}{\rho}\frac{\partial}{\partial x}\left(\frac{q}{\theta}\right).
\end{aligned} \tag{2.4}$$

The first of these,$(2.4)_1$, ensures compatibility of the displacements, $(2.4)_2$ is the balance of linear momentum. Equation $(2.4)_3$ is the balance of energy or the first law of thermodynamics, while $(2.4)_4$ is the second law of thermodynamics.

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If within the bar an interface exists, $x = s(t)$, where the fields suffer a discontinuity then these field quantities must satisfy certain jump conditions across such an interface. These jump conditions are the Rankine-Hugoniot equations, which in this one dimensional setting are

$$
\begin{aligned}
[[v]] &= -\dot{s}[[\gamma]], \\
[[\tau]] &= -\dot{s}\rho[[v]], \\
[[\tau v]] + [[q]] &= -\dot{s}[[\varepsilon]] - \frac{\dot{s}}{2}[[v^2]], \\
\dot{s}\rho[[\eta]] + \left[\left[\frac{q}{\theta}\right]\right] &\leq 0.
\end{aligned}
\tag{2.5}
$$

Here $\dot{s}$ denotes the speed in which the surface of discontinuity propagates, $\dot{s} = \frac{d}{dt}s(t)$. The square brackets denotes the jump in the enclosed quantity, say f, across s(t): $[[f]] = f(s^+) - f(s^-)$; while $\langle\langle f\rangle\rangle$ is the average of the function f across the interface: $\langle\langle f\rangle\rangle = \frac{1}{2}[f(s^+) + f(s^-)]$.

The class of problems to be investigated is now restricted to those which describe adiabatic motions, in so doing the internal energy production r and the heat flux q are required to vanish. One may regard adiabatic motions as idealized processes which occur quickly with respect to the continuum thermodynamic time scales associated with the transfer of heat by diffusion and radiation. Isothermal motions may be considered to occupy the other end of the spectrum, where events occurs so slowly that the body has enough time for the transfer of heat such that the temperature can equilibrate with an external ambient temperature. Under the adiabatic assumption, the equations of motion ar

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and jump conditions simplify into the final form which will be used throughout the remainder of this document:

$$\begin{aligned} &\frac{\partial\gamma}{\partial t} = \frac{\partial v}{\partial x}, \\ &\rho\frac{\partial v}{\partial t} = \frac{\partial\tau}{\partial x}, \\ &\frac{d\varepsilon}{dt} = \tau\frac{\partial v}{\partial x}, \\ &\frac{d\eta}{dt} \geq 0, \end{aligned} \tag{2.6}$$

$$\begin{aligned} &[[v]] + \dot{s}[[\gamma]] = 0, \\ &[[\tau]] + \dot{s}\rho[[v]] = 0, \\ &\dot{s}([[\varepsilon]] - \langle\langle\tau\rangle\rangle[[\gamma]]) = 0, \\ &\dot{s}\rho[[\eta]] \leq 0. \end{aligned} \tag{2.7}$$

When working within the context of the mechanics of solids it is often convenient to utilize the Helmholtz free energy function $\psi(\gamma, \theta)$. The internal energy and Helmholtz free energy are not independent, but are related through the expression

$$\varepsilon = \psi + \theta\eta. \tag{2.8}$$

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From standard thermodynamic definitions (Ziegler 1988, Ericksen 1993) the stress and entropy may be derived from the Helmholtz free energy

$$\tau = \frac{\partial\psi}{\partial\gamma}, \qquad \eta = -\frac{\partial\psi}{\partial\theta}. \tag{2.9}$$

From (2.8) the left hand side of $(2.6)_3$ can be expressed $\frac{d\varepsilon}{dt} = \frac{d\psi}{dt} + \frac{d}{dt}(\theta\eta)$, which from the definitions (2.9) and $(2.6)_1$ is simplified $\frac{d\varepsilon}{dt} = \tau\frac{\partial v}{\partial x} + \theta\frac{\partial\eta}{\partial t}$. Therefore the first law of thermodynamics $(2.6)_3$ in the adiabatic setting can be expressed in the alternative fashion

$$\frac{\partial\eta}{\partial t} = 0, \tag{2.10}$$

which requires a particle's entropy to remain constant.

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3. Material Model

3.1 Construction of the Material Response Functions

The purely mechanical problem of a packet of shear waves interacting with a phase boundary has been previously studied (Pence 1991a, 1991b). However during such processes a more complete description necessitates accounting for thermal as well as mechanical effects (James 1983,Truskinovsky 1985). Recently, a material model has been developed which may be used to describe a multi-phase thermoelastic solid (Abeyaratne and Knowles 1992c). The model considered in this document is similar in form to theirs, but we more fully use its ability to model thermomechanical motions by less simplification of material parameters. One major goal of this research is to introduce this model and demonstrate its ability of capturing nonlinear elastic adiabatic motions. We also will demonstrate its ability to collapse into a form which is purely mechanical, and for which certain previously determined results are shown to fall under a more complete thermomechanical framework.

The model to be presented intuitively seems more realistic than a description which allows only mechanical motions, and the use of this more complex energetic description should enable one to gain a better understanding of observed physical phenomena such as thermal softening and the Austenite/Martensite transformation, the later being more in the focus of this research. This section explains the model while latter sections modify it, the final form being the basis for the remainder of this work.

Assume the internal energy to be a state function with thermodynamic variables of temperature and strain. For a linear elastic stress strain response, the internal energy ε

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should be a quadratic function in strain γ at constant temperature θ:

$$\varepsilon = \tilde{\varepsilon}(\gamma, \theta) = \frac{1}{2}\mu(\theta)\,[\gamma - a(\theta)]^2 + b(\theta)\,. \tag{3.1}$$

Here and throughout this manuscript the tilde superscript will be used to indicate a functional dependance on strain γ and temperature θ. From this initial form of the internal energy we will construct the Helmholtz free energy from which the stress and entropy may be derived. An alternative approach is to begin with the internal energy using the strain and entropy as the appropriate thermodynamic variables from which the stress and temperature follow. In this setting, any material whose internal energy can be additively decomposed into a function of strain alone and a function of entropy alone will be referred to as *separable*. This special form of the internal energy ensures that the stress is independent of the entropy and results in the mechanical jump conditions $(2.5)_{1,2}$ being independent from the energy jump condition $(2.5)_3$. Knowledge of this special form for the internal energy function will prove useful in future development within this document.

From (2.9) the Helmholtz free energy ψ can be expressed

$$\psi = \tilde{\psi}(\gamma, \theta) = \tilde{\varepsilon} - \theta\tilde{\eta}, \tag{3.2}$$

where $\tilde{\eta}(\gamma, \theta)$, the entropy of the material, is also a function of strain and temperature. The entropy can be developed by using the following results from (3.2) and (2.9)

$$-\tilde{\eta} = \frac{\partial}{\partial\theta}\tilde{\psi} = \frac{\partial}{\partial\theta}\tilde{\varepsilon} - \tilde{\eta} - \theta\frac{\partial}{\partial\theta}\tilde{\eta}. \tag{3.3}$$

By manipulating equations (3.1)-(3.3) the following expression for the entropy is found

$$\frac{\partial}{\partial\theta}\tilde{\eta} = \frac{1}{\theta}\frac{\partial}{\partial\theta}\tilde{\varepsilon} = \frac{1}{\theta}\left[\frac{\mu'(\theta)}{2}[\gamma - a(\theta)]^2 - \mu(\theta)\,[\gamma - a(\theta)]\,a'(\theta) + b'(\theta)\right], \tag{3.4}$$

here the superimposed prime denotes differentiation with respect to the function's lone variable.

Equation (3.4) may be integrated thereby giving the entropy to within an arbitrary function of the strain

$$\tilde{\eta}(\gamma,\theta) = \int^{\theta} \left[\frac{\mu'(\xi)}{2}[\gamma - a(\xi)]^2 - \mu(\xi)\,[\gamma - a(\xi)]\,a'(\xi) + b'(\xi)\right]\frac{d\xi}{\xi} + F(\gamma)\,, \tag{3.5}$$

where $F(\gamma)$ resulting from the integration is a function of the strain γ only. Combining the internal energy (3.1) and the entropy (3.5) to construct the free energy (3.2) one may then calculate the stress via definition $(2.9)_1$

$$\tilde{\tau}(\gamma,\theta) = \mu(\theta)\,[\gamma - a(\theta)]\, - \tag{3.6}$$

$$\theta\int^{\theta} [\mu'(\xi)\,[\gamma - a(\xi)] - \mu(\xi)\,a'(\xi)]\,\frac{d\xi}{\xi} - \theta F'(\gamma)\,,$$

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$$\tilde{\tau}(\gamma, \theta) = \zeta_1(\theta)\gamma + \zeta_2(\theta) - \theta F'(\gamma)\,, \tag{3.7}$$

where

$$\zeta_1(\theta) = \mu(\theta) - \theta\int^{\theta} \mu'(\xi)\frac{d\xi}{\xi}, \tag{3.8}$$

$$\zeta_2(\theta) = -\mu(\theta)\,a(\theta) + \theta\int^{\theta} \mu'(\xi)\,a(\xi)\frac{d\xi}{\xi} + \theta\int^{\theta} \mu(\xi)\,a'(\xi)\frac{d\xi}{\xi}. \tag{3.9}$$

The following restrictions are now placed on the response functions so that certain desirable features may be incorporated into the material model. These assumptions are guided by the desire for a model with enough generality to capture the phenomena of interest in a mathematically tractable fashion.

(A1) The slope of the stress-strain curve is independent of temperature.

(A.2) The internal energy has a linear dependance on the temperature at constant strain.

Formally the restriction (A1) states: $\frac{\partial^2}{\partial\theta\partial\gamma}\tilde{\tau}(\gamma, \theta) = 0$. Carrying out this differentiation using equations (3.7) and(3.8) leads to

$$\frac{d^2}{d\gamma^2}F(\gamma) = \zeta_1'(\theta) = \chi = \text{constant.} \tag{3.10}$$

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After performing the necessary integration, the expression for $F(\gamma)$ is found to be:

$$F(\gamma) = \frac{\chi\gamma^2}{2} + \bar{k}\gamma + \hat{k}. \tag{3.11}$$

Equations (3.8) and (3.10) yield: $\chi = \zeta'_1(\theta) = \frac{\partial}{\partial\theta}\left(\mu(\theta) - \theta\int_{\theta}\mu'(\xi)\frac{d\xi}{\xi}\right)$,where upon rearranging one finds

$$\chi = -\int^{\theta}\mu'(\xi)\frac{d\xi}{\xi}. \tag{3.12}$$

From (3.10)-(3.12)

$$\chi = 0, \qquad \mu(\theta) = \mu = \text{constant}, \qquad F(\gamma) = \bar{k}\gamma + \hat{k}. \tag{3.13}$$

Assumption (A.2) states that $\frac{\partial^2}{\partial\theta^2}\tilde{\varepsilon}(\gamma, \theta) = 0$, so that (3.13) coupled with (3.1) require that the functions $a(\theta)$ and $b(\theta)$ satisfy

$$a(\theta) = a, \qquad b(\theta) = \bar{b}\theta + \hat{b}, \tag{3.14}$$

where a, $\bar{b}$, and $\hat{b}$ are material constants. Inserting expressions (3.13) and (3.14) into equations (3.1), (3.5), and (3.6) for the internal energy, entropy and stress yields

$$\varepsilon = \tilde{\varepsilon}(\gamma, \theta) = \frac{1}{2}\mu(\gamma - a)^2 + \bar{b}\theta + \hat{b}, \tag{3.15}$$

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$$\eta = \tilde{\eta}(\gamma, \theta) = \bar{b} \ln(\theta) + \bar{k}\gamma + \hat{k}, \tag{3.16}$$

$$\tau = \tilde{\tau}(\gamma, \theta) = \mu(\gamma - a) - \bar{k}\theta, \tag{3.17}$$

where a, $\bar{b}$, $\hat{b}$, μ, $\bar{k}$, $\hat{k}$ are constants which characterize the material.

The non-dimensionalization of the argument within the logarithmic function is implicit in the integration of the function F(γ) of $(3.13)_3$. This can be achieved by recognizing that the integration constant $\hat{k}$ may be redefined in any convenient manner. To make this explicit, let $\hat{k} = -\bar{b}\ln(\theta^*) + \tilde{k}$, where the normalization temperature θ^* is

$$\theta^* \equiv \exp\left(\frac{\tilde{k} - \hat{k}}{\bar{b}}\right). \tag{3.18}$$

This temperature will be defined more precisely in later sections of the document. The logarithmic function in the entropy (3.16) can now be normalized using (3.18)

$$\tilde{\eta}(\gamma, \theta) = \bar{b}\ln\left(\frac{\theta}{\theta^*}\right) + \bar{k}\gamma + \tilde{k}. \tag{3.19}$$

The constant $\tilde{k}$ is then by definition $\tilde{k} = \hat{k} + \bar{b}\ln(\theta^*)$, a physical interpretation of $\tilde{k}$ is ambiguous, from (3.19) one might think of it as the low entropy limit. For notational ease, the constant a in (3.14), and contained in both the internal energy (3.15) and stress (3.17), will be defined as:

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$$a \equiv \gamma^* - \frac{\bar{k}\theta^*}{\mu}. \tag{3.20}$$

Using this slight modification of the material parameters the Helmholtz free energy can be written from its defintion (3.2) and equations (3.15), (3.19), and (3.20) as

$$\psi(\gamma, \theta) = \frac{\mu}{2}\left[\gamma - \left(\gamma^* - \frac{\bar{k}\theta^*}{\mu}\right)\right]^2 + \bar{b}\theta\left[1 - \ln\left(\frac{\theta}{\theta^*}\right)\right] - \bar{k}\theta\gamma - \tilde{k}\theta + \hat{b}. \tag{3.21}$$

The stress reduces to

$$\tilde{\tau}(\gamma, \theta) = \frac{\partial}{\partial\gamma}\psi(\gamma, \theta) = \mu(\gamma - \gamma^*) - \bar{k}(\theta - \theta^*). \tag{3.22}$$

In both (3.21) and (3.22) the term γ^* appears, it is an "offset" strain whose role will become more apparent later in this document.

The constitutive model for the material may now be utilized in the dynamical balance equations (2.6), which yield

$$\frac{\partial\gamma}{\partial t} = \frac{\partial v}{\partial x}, \tag{3.23}$$

$$\rho\frac{\partial v}{\partial t} = \mu\frac{\partial\gamma}{\partial x} - \bar{k}\frac{\partial\theta}{\partial x}, \tag{3.24}$$

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$$\mu\left[\gamma-\left(\gamma^{*}-\frac{\bar{k}\theta^{*}}{\mu}\right)\right]\frac{\partial\gamma}{\partial t}+\bar{b}\frac{\partial\theta}{\partial t} = \left[\mu(\gamma-\gamma^{*})-\bar{k}(\theta-\theta^{*})\right]\frac{\partial v}{\partial x}, \tag{3.25}$$

$$\frac{\bar{b}\partial\theta}{\theta\partial t}+\bar{k}\frac{\partial\gamma}{\partial t}\geq 0. \tag{3.26}$$

The above development has shown that (3.15)-(3.19) is the most general constitutive model for an energy function of the form (3.1) subject to assumptions (A.1) and (A.2).

The material parameters $\mu, \gamma^{*}, \theta^{*}, \bar{b}, \hat{b}, \bar{k}, \tilde{k}$, which arose naturally in the construction of the above model, can be interpreted in terms of measurable thermodynamic parameters. First, (3.22) gives that $\mu = \frac{\partial^2\psi}{\partial\gamma^2}$ and so μ is the isothermal elastic modulus, which is considered a positive quantity. Second, the *specific heat* for constant strain C_γ is defined (Truesdell and Toupin 1960) as

$$C_\gamma \equiv \frac{\theta}{\rho}\left(\frac{\partial\eta}{\partial\theta}\right)_\gamma = -\frac{\theta}{\rho}\frac{\partial^2\tilde{\psi}}{\partial\theta^2}, \tag{3.27}$$

so that (3.16) gives

$$C_\gamma = \frac{\bar{b}}{\rho}. \tag{3.28}$$

Thus $\bar{b} = \rho C_\gamma$ is a material parameter analogous to the materials specific heat, the heat capacity, and is also a positive quantity. Third, the constant $\bar{k}$ may be interpreted in a similar manner since (3.17) allows us to write the strain as a function of stress and temperature

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$$\gamma(\tau, \theta) = \gamma^* + \frac{\tau}{\mu} + \frac{\bar{k}(\theta - \theta^*)}{\mu}. \tag{3.29}$$

Choosing as a reference state $\tau = 0, \theta = \tilde{\theta}$ it follows from (3.29) that if the stress free state persists for temperatures above the reference temperature $\tilde{\theta}$, then there will occur a proportional increase in the strain, $\gamma(0, \theta) - \gamma(0, \tilde{\theta}) = \frac{\bar{k}(\theta - \tilde{\theta})}{\mu}$. Thus the quantity $\bar{k}/\mu$ is the material's coefficient of thermal expansion, which is, in general, a positive quantity. If we denote the coefficient of thermal expansion as α, then

$$\alpha = \frac{\bar{k}}{\mu}. \tag{3.30}$$

By definition (Truesdell and Toupin 1960) the coefficient of thermal expansion is written $\alpha \equiv \left.\frac{\partial\gamma}{\partial\theta}\right|_{\tau}$, performing the prescribed differentiation on (3.28) also yields (3.30). In terms of various derivatives of the material's free energy, the coefficient of thermal expansion can be expressed as $\alpha = -\frac{1}{\mu}\frac{\partial^2\psi}{\partial\gamma\partial\theta}$.

The parameter $\hat{b}$ interpretation is that of a contribution to the internal energy's "base level". For constant temperature the vertex of $\varepsilon(\gamma, \theta)$ is located at $\gamma = a$, which may be expressed somewhat more precisely using (3.20), the value of the energy at this particular temperature and strain is $\bar{b}\theta + \hat{b}$. Thus $\hat{b}$ is always an additional contribution to the internal energy's base level at temperature θ, and one could let this quantity vanish without much loss in the model.Table 1 consolidates the above information for the material constants $\mu, \gamma^*, \theta^*, \bar{b}, \hat{b}, \bar{k}, \tilde{k}$ and provides dimensional information for these constants.

Table 1: Material parameters

Material Constant	Units in terms of [mass], [length], [time], [temperature]	Physical Interpretation
μ	$\dfrac{[\text{mass}]}{[\text{length}]\,[\text{time}]^2}$	Isothermal elastic modulus.
γ^*	$\dfrac{[\text{length}]}{[\text{length}]}$	The relaxed ($\tau = 0$) strain when $\theta = \theta^*$.
θ^*	[temperature]	Normalization temperature which can be chosen as convenient.
$\bar{b}$	$\dfrac{[\text{mass}]}{[\text{length}]\,[\text{temperature}]\,[\text{time}]^2}$	Heat capacity.
$\hat{b}$	$\dfrac{[\text{mass}]}{[\text{length}]\,[\text{time}]^2}$	The ground state for the internal energy.
$\bar{k}$	$\dfrac{[\text{mass}]}{[\text{length}]\,[\text{temperature}]^2\,[\text{time}]^2}$	Product of the isothermal elastic modulus and coefficient of thermal expansion.
$\tilde{k}$	$\dfrac{[\text{mass}]}{[\text{length}]\,[\text{temperature}]^2\,[\text{time}]^2}$	Value of entropy when $\theta = \theta^*$ and $\gamma = 0$.

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It will henceforth be convenient to abandon the parameters $\tilde{b}$, $\tilde{k}$ which arose naturally in the model's development, in favor of the more common thermodynamic parameters C_γ and α. The free energy, entropy and stress are written out below utilizing these parameters

$$\psi(\gamma,\theta) = \frac{\mu}{2}(\gamma-(\gamma^*-\alpha\theta^*))^2+\rho C_\gamma\theta\left[1-\ln\left(\frac{\theta}{\theta^*}\right)\right]-\mu\alpha\theta\gamma-\tilde{k}\theta+\hat{b},$$

$$\tilde{\eta}(\gamma,\theta) = \rho C_\gamma \ln\left(\frac{\theta}{\theta^*}\right)+\mu\alpha\gamma+\tilde{k}, \qquad (3.31)$$

$$\tilde{\tau}(\gamma,\theta) = \mu(\gamma-\gamma^*)-\mu\alpha(\theta-\theta^*).$$

The reader is reminded that θ^* is essentially a free parameter in this description since any redefinition of the value for θ^* can be compensated for by a redefinition of the values $\tilde{k}$ and γ^* by

$$\begin{gathered}\theta^*_{\mathrm{old}}\rightarrow\theta^*_{\mathrm{new}}\Rightarrow\tilde{k}_{\mathrm{old}}\rightarrow\tilde{k}_{\mathrm{old}}+\rho C_\gamma\ln\left(\frac{\theta^*_{\mathrm{new}}}{\theta^*_{\mathrm{old}}}\right)\equiv\tilde{k}_{\mathrm{new}}, \\ \gamma^*_{\mathrm{old}}\rightarrow\gamma^*_{\mathrm{old}}-\alpha\left(\theta^*_{\mathrm{old}}-\theta^*_{\mathrm{new}}\right)\equiv\gamma^*_{\mathrm{new}}.\end{gathered} \qquad (3.32)$$

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3.2 Separable Energy

In the above analysis we have chosen to use the stain γ and temperature θ as the relevant thermodynamic variables, whereas in a more traditional thermomechanical analysis one would work with the strain γ and entropy η as the independent variables. We now recast the above model in terms of the strain and entropy, then the internal energy, (3.15) may be expressed

$$\tilde{\varepsilon}(\gamma,\theta) = \tilde{\varepsilon}(\gamma,\hat{\theta}(\gamma,\eta)) = \hat{\varepsilon}(\gamma,\eta), \tag{3.33}$$

assuming that one may invert the entropy function $\tilde{\eta}(\gamma,\theta)$ for the temperature: $\theta = \hat{\theta}(\gamma,\eta)$. Using (3.16) one finds that the temperature as a function of strain and entropy is given by

$$\ln\left(\frac{\theta}{\theta^*}\right) = \frac{\eta-\mu\alpha\gamma-\tilde{k}}{\rho C_\gamma},$$

where upon inverting

$$\hat{\theta}(\gamma,\eta) = \theta^*\exp\left(\frac{\eta-\mu\alpha\gamma-\tilde{k}}{\rho C_\gamma}\right). \tag{3.34}$$

Thus by substituting from equation (3.34) into (3.33), the internal energy may be expressed as a function of the strain and entropy. An analogous procedure can be performed on the stress, the results of these operations gives

$$\varepsilon = \hat{\varepsilon}(\gamma, \eta) = \frac{\mu}{2}(\gamma - (\gamma^* - \alpha\theta^*))^2 + \rho C_\gamma \theta^* \exp\left(\frac{\eta - \mu\alpha\gamma - \tilde{k}}{\rho C_\gamma}\right) + \hat{b}, \tag{3.35}$$

$$\tau = \hat{\tau}(\gamma, \eta) = \mu(\gamma - \gamma^*) - \mu\alpha\theta^* \left[\exp\left(\frac{\eta - \mu\alpha\gamma - \tilde{k}}{\rho C_\gamma}\right) - 1\right]. \tag{3.36}$$

Equation (3.35) demonstrates that if the coefficient of thermal expansion α vanishes $(\alpha \to 0)$ then the internal energy can be written as the additive combination of a function of the strain alone and a function of the entropy alone, i.e.

$$\hat{\varepsilon}(\gamma, \eta) = \frac{\mu}{2}(\gamma - \gamma^*)^2 + \rho C_\gamma \theta^* \exp\left(\frac{\eta - \tilde{k}}{\rho C_\gamma}\right) + \hat{b} \qquad (\alpha = 0). \tag{3.37}$$

Recall that (3.37) is the special form of the internal energy that we termed separable in Section 3.1. If the internal energy is separable then the equations governing the mechanical evolution of the body are independent of those controlling the thermal evolution (Courant and Freidrichs 1956). Since this decoupling between thermal and mechanical processes will play a significant role in this research, we temporarily proceed by developing the associated material response functions under this specialization. Setting $\alpha = 0$ the stress and temperature reduce to

$$\begin{aligned} \hat{\tau}(\gamma) &= \frac{\partial}{\partial\gamma}\hat{\varepsilon}(\gamma, \eta) = \mu(\gamma - \gamma^*), \\ \theta(\eta) &= \frac{\partial}{\partial\eta}\hat{\varepsilon}(\gamma, \eta) = \theta^* \exp\left(\frac{\eta - \tilde{k}}{\rho C_\gamma}\right). \end{aligned} \qquad (\alpha = 0) \tag{3.38}$$

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In this specialized form the equations of motion (3.23)-(3.25) reduce to

$$\frac{\partial \gamma}{\partial t} = \frac{\partial v}{\partial x} \qquad (\alpha = 0)\,, \tag{3.39}$$

$$\rho\frac{\partial v}{\partial t} = \mu\frac{\partial \gamma}{\partial x} \qquad (\alpha = 0)\,, \tag{3.40}$$

$$\theta^{*}\exp\left(\frac{\eta - \tilde{k}}{\rho C_{\gamma}}\right)\frac{\partial \eta}{\partial t} = 0 \qquad (\alpha = 0)\,. \tag{3.41}$$

Since the normalization temperature θ^{*} need not vanish, one draws $\theta^{*}\exp\left(\frac{\eta - \tilde{k}}{\rho C_{\gamma}}\right) \neq 0$ and (3.41) reduces to

$$\frac{\partial \eta}{\partial t} = 0 \qquad (\alpha = 0)\,, \tag{3.42}$$

which, when coupled with (3.38), gives rise to

$$\frac{\partial \theta}{\partial t} = 0 \qquad (\alpha = 0)\,. \tag{3.43}$$

Thus, in the absence of discontinuities such as shocks, (3.43) shows that boundary value problems which have isothermal initial conditions will proceed isothermally. Furthermore, considering this special $(\alpha = 0)$ case, the entropy for each particle will persist from the initial state.

From (3.39)-(3.41), it is seen that if the internal energy is separable, then the governing equations for the body simplify into two distinct sets of governing equations, one being (3.39) and (3.40), which are a purely mechanical in nature, i.e. they only involve the velocity and strain fields, the other set is (3.42), which governs the thermal evolution within the body. For materials with such a separable energy one could envision boundary value problems in which a specific thermomechanical problem is posed and from the above results we see that the mechanical fields develop independently of the thermal fields. For such boundary value problems, the mechanical fields being independent of the thermal fields, the investigation can completely ignore the thermal evolution which occurs and concentrate on the purely mechanical problem.

3.3 Characteristics and Riemann Invariants

It is observed that the governing equations(3.23)-(3.25) are a system of homogeneous quasi-linear first order partial differential equations in terms of the three independent field quantities: v , γ and θ . One may derive a different yet equivalent set of governing equations by use of the method of characteristics (Renardy and Rogers 1992). This technique yields an alternative set of governing equations which are linear combinations of the original system of equations, such that the dependent variables in each resulting equation are differentiated in the same direction in the (x,t)-plane. The directions of differentiation are called the characteristic directions or *characteristics* of the system, and the alternative equations are the *characteristic equations* of the system. In general this met

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method of construction (Renardy and Rogers 1992) proceeds as outlined in the next paragraphs.

Consider a system of first order partial differential equations written in the form

$$AU_x + BU_t = C. \tag{3.44}$$

where the column vector U consists of the unknown functions to be determined, and A, B, and C are the coefficient matrices, which may be functions of x, t, and the components of the vector U, but not U_x or U_t. In this study $U = [\gamma, v, \theta]^T$. The characteristic directions and equations for (3.44) are obtained from the solutions to the eigenvalue problem

$$\Lambda^T (A - \lambda B) = 0, \tag{3.45}$$

where the scalars λ are the eigenvalues for the above problem, and the column vectors Λ are the left eigenvectors for the system. The eigenvalues λ are the characteristic directions for the original system of equations

$$\frac{dx}{dt} = \lambda. \tag{3.46}$$

For each eigenvalue the associated eigenvector Λ is used to determine the characteristic equation by forming linear combinations of the original system in the form

$$\Lambda^T A U_x + \Lambda^T B U_t = \Lambda^T C, \tag{3.47}$$

where the dependent variables in the resulting equation are all differentiated in the same direction, the directional derivatives being the characteristic directions of the system.

3.3.1 Separable Materials

We begin by considering the method of characteristics for a material having a separable energy. We use our original set of PDE's (3.23)-(3.25), setting $\alpha = 0$, the governing equations are then

$$\begin{aligned} \frac{\partial\gamma}{\partial t} &= \frac{\partial v}{\partial x} \\ \rho\frac{\partial v}{\partial t} &= \mu\frac{\partial\gamma}{\partial x} \qquad\qquad (\alpha = 0) \\ \mu(\gamma-\gamma^*)\frac{\partial\gamma}{\partial t} + \rho C_\gamma\frac{\partial\theta}{\partial t} &= \mu(\gamma-\gamma^*)\frac{\partial v}{\partial x} \end{aligned} \tag{3.48}$$

Analyzing the system of equations (3.48) it is not immediate that the mechanical field quantities are decoupled form the thermal field quantities. However, by recasting the system of equations using the method of characteristics, the temperature is shown to decouple from the strain and velocity. Proceeding with the method of characteristics for the above case in which $\alpha = 0$, produces an alternative system of governing equations, the characteristic equations and the characteristic directions of the original system. Written in matrix form as in (3.44), where the vector $U = [\gamma, v, \theta]^T$, the governing equations are now

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$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \mu & 0 \\ \mu(\gamma-\gamma^*) & 0 & 0 \end{bmatrix} \begin{bmatrix} v_x \\ \gamma_x \\ \theta_x \end{bmatrix} + \begin{bmatrix} 0 & -1 & 0 \\ -\rho & 0 & 0 \\ 0 & -\mu(\gamma-\gamma^*) & -\rho C_\gamma \end{bmatrix} \begin{bmatrix} v_t \\ \gamma_t \\ \theta_t \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad (\alpha = 0)\,.$$

Performing the calculations described above, the characteristic equations and characteristic directions are found to be:

$$\frac{d\theta}{dt} = 0 \text{ on } \frac{dx}{dt} = 0, \tag{3.49}$$

$$(\alpha = 0)$$

$$\frac{dv}{dt} \mp \sqrt{\frac{\mu}{\rho}} \frac{d\gamma}{dt} = 0 \text{ on } \frac{dx}{dt} = \pm\sqrt{\frac{\mu}{\rho}}. \tag{3.50}$$

The system of equations (3.49)-(3.50) is composed of a characteristic equation, which is the left equation of either set, and the associated characteristic direction, the right equation. Equation (3.49) was to be expected since it was derived in an alternative manner, see (3.42). Along each characteristic direction it follows that the associated characteristic equation may be integrated, providing an algebraic relationship along the characteristic direction

$$\theta = \text{constant on } \frac{dx}{dt} = 0, \tag{3.51}$$

$$(\alpha = 0)$$

$$v \mp \sqrt{\frac{\mu}{\rho}}\gamma = \text{constant on } \frac{dx}{dt} = \pm\sqrt{\frac{\mu}{\rho}}, \tag{3.52}$$

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the constants of integration in the above equations are known in the literature as the *Riemann Invariants* of the system (c.f. Renardy and Rogers 1992). For ease of notation we introduce the material constant

$$c = \sqrt{\mu/\rho}, \tag{3.53}$$

which is the *acoustic wave speed* of the material, this allows (3.39) to be expressed as

$$v \mp c\gamma = \text{constant on } \frac{dx}{dt} = \pm c. \qquad (\alpha = 0) \tag{3.54}$$

Through the use of (3.52) one can calculate the strain and velocity fields independently of the temperature field, and vice-versa. In fact from the above results it is seen that all motions which begin from a constant temperature proceed isothermally, if the formation of shocks are excluded. Thus if $\alpha = 0$ then the mechanical and thermal evolution of the material proceeds independently of one another.

Consider an initial-boundary value problem such that the above set of characteristic equations hold. If the initial-boundary data is given then the Riemann invariants can be calculated along the associated characteristic directions. One could then proceed with the initial-boundary value problem and formulate a set of algebraic equations relating the Riemann invariants in different regions within the domain, where the different regions are connected along one or more of the associated characteristic directions. Pence in his investigations (1991a,b) demonstrated the use of this technique in formulating families of solutions for a set of problems under this purely mechanical framework.

3.3.2 Nonseparable Materials

Consider now the more general problem in which the thermal-mechanical responses are coupled, from the earlier development this occurs when the coefficient of thermal expansion does not vanish, $\alpha \neq 0$. The method of characteristics will now be developed for this case. The equations of motion in terms of field variables $\gamma(x, t)$, $\theta(x, t)$ and $v(x, t)$ are found by inserting the constitutive response,(3.15)-(3.21), into (3.23)-(3.25), and using (3.53)

$$\frac{\partial \gamma}{\partial t} = \frac{\partial v}{\partial x}, \tag{3.55}$$

$$c^2\frac{\partial \gamma}{\partial x} - c^2\alpha\frac{\partial \theta}{\partial x} = \frac{\partial v}{\partial t}, \tag{3.56}$$

$$c^2(\gamma - (\gamma^* - \alpha\theta^*))\frac{\partial \gamma}{\partial t} + C_\gamma\frac{\partial \theta}{\partial t} = c^2((\gamma - \gamma^*) - \alpha(\theta - \theta^*))\frac{\partial v}{\partial x}. \tag{3.57}$$

The first step in finding the characteristic directions and equations is to cast (3.55)-(3.57) in matrix form

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & c^2 & -c^2\alpha \\ c^2((\gamma-\gamma^*)-\alpha(\theta-\theta^*)) & 0 & 0 \end{bmatrix} \begin{bmatrix} v_x \\ \gamma_x \\ \theta_x \end{bmatrix} + \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & -c^2(\gamma-(\gamma^*-\alpha\theta^*)) & -C_\gamma \end{bmatrix} \begin{bmatrix} v_t \\ \gamma_t \\ \theta_t \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \tag{3.58}$$

as before the characteristic directions and equations as well as the eigenvalues and eigenvectors for are to be determined. Performing the necessary calculations one finds that the characteristic equations and directions are

$$c^2\alpha\frac{d\gamma}{dt}+\frac{C_\gamma}{\theta}\frac{d\theta}{dt} = 0 \text{ on } \frac{dx}{dt} = 0, \tag{3.59}$$

$$\pm\sqrt{c^2+\frac{c^4\alpha^2\theta dv}{C_\gamma\, dt}}+c^2\frac{d\gamma}{dt}-c^2\alpha\frac{d\theta}{dt} = 0 \text{ on } \frac{dx}{dt} = \mp c\sqrt{1+\frac{c^2\alpha^2\theta}{C_\gamma}}. \tag{3.60}$$

Equation (3.59) is equivalent to requiring that a particle's entropy remain unchanged during smooth processes. This can be shown by differentiating equation (3.16) with respect to time and comparing the result with

$$\frac{d\eta}{dt} = \frac{\rho C_\gamma}{\theta}\frac{d\theta}{dt}+\rho c^2\alpha\frac{d\gamma}{dt} = 0 \text{ on } \frac{dx}{dt} = 0. \tag{3.61}$$

One can integrate the expression (3.61) along its characteristic direction and arrive at the conclusion that a particle's entropy is conserved along its characteristic direction. This constant would be one of the Riemann invariants for this thermomechanical problem, i.e.

$$\eta = \tilde{\eta}(\gamma,\theta) = \rho C_\gamma \ln\left(\frac{\theta}{\theta_*}\right)+\rho c^2\alpha\gamma+\tilde{k} = \text{constant on } \frac{dx}{dt} = 0. \tag{3.62}$$

The wave speed in (3.60) is no longer constant, as in (3.52), but now is dependent on the material's temperature. It is seen that the wave speed is a monotonically increasing function of the temperature for the model under consideration here. In general equations (3.60) and (3.46) cannot be integrated, and hence the other two Riemann invariants are not known in advance. However, it is possible to calculate these two Riemann invariants if the initial data are specified in a particular manner. Since the knowledge of these invariants will enable us to construct a solution to the problem defined in Chapter 6, the discussion of this special case will be pursued in the following paragraphs.

Consider the problem just outlined above and in addition suppose that the entropy is initially constant on a region contained within the domain. As a result of equation (3.62) the entropy within this region is constant for all time. Under these assumptions we may manipulate (3.61) and find a relationship between γ and θ in this same region

$$\frac{d\gamma}{dt} = -\frac{C_\gamma}{c^2\alpha\theta}\frac{d\theta}{dt} \text{ on } \frac{dx}{dt} = 0. \tag{3.63}$$

Since η does not vary in the region for all time we can substitute from (3.63) into equations (3.60), resulting in

$$\pm\sqrt{c^2 + \frac{c^4\alpha^2\theta}{C_\gamma}}\frac{dv}{dt} - \frac{C_\gamma}{\theta c^2\alpha}\left[c^2 + \frac{c^4\alpha^2\theta}{C_\gamma}\right]\frac{d\theta}{dt} = 0 \text{ on } \frac{dx}{dt} = \mp c\sqrt{1 + \frac{c^2\alpha^2\theta}{C_\gamma}}. \tag{3.64}$$

The two equations (3.64) may now be integrated along their characteristic directions to produce two additional Riemann invariants, the results of which are shown below:

$$\pm v - \sqrt{C_\gamma}\left[2\Phi(\theta) + \Phi(0)\ln\left(\frac{\Phi(\theta) - \Phi(0)}{\Phi(\theta) + \Phi(0)}\right)\right] = \text{constant}, \tag{3.65}$$

on

$$\frac{dx}{dt} = \mp c\sqrt{1 + \frac{c^2\alpha^2\theta}{C_\gamma}}, \tag{3.66}$$

where

$$\Phi(\theta) = \sqrt{\theta + \frac{C_\gamma}{c^2\alpha^2}}. \tag{3.67}$$

In general, if the assumption of constant entropy is not met, then integration of equations (3.64) is not possible and the results (3.65) need not hold.

The form of the characteristic speed in (3.66) shows that it is monotonically increasing with temperature θ and coincident with the isothermal sound speed only in the limit $\theta \to 0$. This can be viewed as the adiabatic correction to a purely mechanical isothermal theory (in which the sound speed is formally temperature independent). Presumably an adiabatic correction to an isothermal theory with a temperature dependent sound speed would behave similarly. A familiar example is provided by flow in a compressible fluid (Landau and Lifshitz (1987), Whitham (1974)), where the sound speed is, in general, given by $\sqrt{\frac{dp}{d\rho}}$ where p is pressure and ρ is density. For a polytropic gas, the sound speed in an isothermal setting follows from the ideal gas law $p = R\rho\theta$, where R is the ideal gas constant, as $c \equiv \sqrt{R\theta}$. For adiabatic conditions, the entropy $C_v \ln\left(\frac{p}{\rho^l}\right)$ is constant, where $l = C_p/C_v = 1 + R/C_v$, C_p and C_v give the specific heats at constant pressure and volume. This gives the adiabatic sound speed as $\sqrt{\frac{lp}{\rho}} = \sqrt{lR\theta} \equiv c_{\text{adiabatic}}$. Thus $c_{\text{adiabatic}} = c\sqrt{1 + \frac{R^2\theta}{C_v c^2}}$, which displays a similar temperature dependance to the adiabatic correction of isothermal sound speed.

3.4 Multiphase Materials

We now broaden the class materials considered to those which allow for the existence of different phases and the transformation between phases. At each point within the body the material is said to occupy a phase, this being determined by the value of strain and temperature at that location. In light of the previous derivations, consider a multiphase material for which each distinct phase can be modeled using the Helmholtz free energy function (3.21) developed earlier in this chapter. For first order phase transitions it is required that the free energy be a continuous function of strain and temperature, but its derivatives may suffer discontinuities. Begin the construction of the multiphase model by assuming that the internal energy, stress, entropy, and free energy functions in any phase has the form as provided by equations (3.15)-(3.21). Assume for generality that there are n possible phases and that from (3.21) the free energy in phase i is

$$\tilde{\psi}_i(\gamma, \theta) = \frac{\rho c_i^2}{2}\left[\gamma - (\gamma_i^* - \alpha_i\theta^*)\right]^2 + \rho C_{\gamma i}\theta\left[1 - \ln\left(\frac{\theta}{\theta^*}\right)\right] - \rho c_i^2\alpha_i\theta\gamma - \tilde{k}_i\theta + \hat{b}_i. \quad (3.68)$$

Thus each phase is characterized by material constants c_i, γ_i^*, $\bar{b}_i$, $\hat{b}_i$, $\bar{k}_i$, $\tilde{k}_i$, and the normalized temperature θ^* is chosen to be the same for all phases. The relations (3.32) between

the material parameters $\tilde{k}$, γ^* and θ^*, ensures that there is a no loss in generality in requiring θ^* to be the same for all phases. A slightly modified form of the free energy (3.68) can be written which displays its "potential well" structure

$$\tilde{\psi}_i(\gamma,\theta) = \frac{\rho c_i^2}{2}\left[\gamma - (\gamma_i^* + \alpha_i(\theta - \theta^*))\right]^2 + \rho C_{\gamma i}\theta\left[1 - \ln\left(\frac{\theta}{\theta^*}\right)\right] - \frac{\rho c_i^2 \alpha_i^2}{2}(\theta - \theta^*)^2 \quad (3.69)$$

$$-(\rho c_i^2 \alpha_i \gamma_i^* + \tilde{k}_i)\theta + \frac{\rho c_i^2 (\alpha_i \theta^*)^2}{2} + \hat{b}_i .$$

At a fixed temperature θ it is seen from (3.69)that the free energy is a quadratic function in strain γ, and the associated energy $\tilde{\psi}_i(\gamma,\theta)$ may be thought of as a "potential well", whose strain-vertex is located at $\gamma = \gamma_i^* + \alpha_i(\theta - \theta^*)$. The location of each of these vertices changes as the temperature varies (the wells movie up and down). By definition a first order phase transformation process that advances through equilibrium states requires that the free energy be a continuous function during the phase transition. Therefore for a first order equilibrated transformation, say between phase-i and phase-j, it is required that $\tilde{\psi}_i - \tilde{\psi}_j = 0$.

Consider a material which has n phases, then at each set of temperature and strain, (γ,θ), there are n values of the free energy $\tilde{\psi}_i(\gamma,\theta)$ i=1,...,n. The minimum value of the collection of free energies $\tilde{\psi}_i$ defines the energy minimal phase-i associated with the pair (γ,θ). This energy minimum implies a phase indicator function I, where

$$(I \in [1, \dots, n] = I(\gamma,\theta)),$$

$$I(\gamma,\theta) \ni \tilde{\psi}_{I(\gamma,\theta)}(\gamma,\theta) = \min_{i = 1,\dots,n}\tilde{\psi}_i(\gamma,\theta) .$$

From this discussion it is evident that a particular set (γ, θ) exists for which two distinct phase's free energies will have equal values. The collection of these sets may be thought of as curves in the (γ, θ) plane where the different phase's free energy functions intersect. This gives rise to an intersection strain,$\tilde{\gamma}_{i,j} = \tilde{\gamma}_{i,j}(\theta)$, the strain $\tilde{\gamma}_{i,j}(\theta)$ at temperature θ where the free energy between phase i and j have the same value. One may think of this as that level of strain where the potential wells intersect. This intersection of free energies naturally leads to a method of determining which phase a material would inhabit given a value of (γ, θ). If one considers the principle of energy minimization as the criterion for selection between two phases, the intersection strain indicates that point in (γ, θ) where two phases would exchange favorably, and the possibility of a phase change exists.

For the material represented by (3.69) two distinct possibilities for $\tilde{\gamma}_{i,j}(\theta)$ exist: one in which $c_i \neq c_j$ and that for which $c_i = c_j$. When such intersections exist, the former case, in general, yields two roots for the intersection strain, while the later yields a single root. This discrepancy between the number of roots is simple to understand. Recall for a fixed temperature that the free energy is a quadratic function of strain, and when the wave speeds are not equal then the curvatures of the two free energy functions are not equal. Because these curvatures are not the same, the quadratic nature of the two free energies functions gives rise to intersections which occur at two different locations (real roots) or which do not intersect at all (imaginary roots). However, when the wave speeds are the same, and thus the curvatures are equivalent, then there is at most one location where the two free energies intersect.

A direct calculation yields the two intersection strains for $c_i \neq c_j$

$$\tilde{\gamma}_{i,j}(\theta) = \frac{-\hat{\Xi}(\theta)}{(c_i^2 - c_j^2)} \pm \frac{\left(\rho^2 \hat{\Xi}^2(\theta) - \widehat{\Xi}(\theta)\right)^{\frac{1}{2}}}{2\rho(c_i^2 - c_j^2)}, \tag{3.70}$$

where

$$\hat{\Xi}(\theta) = (c_j^2 \gamma_j^* - c_i^2 \gamma_i^* + (\alpha_j c_j^2 - \alpha_i c_i^2)(\theta - \theta^*)),$$

$$\widehat{\Xi}(\theta) = 4\rho(c_i^2 - c_j^2)\Big(2(\hat{b}_i - \hat{b}_j) + \rho(c_i^2 \gamma_i^* - c_j^2 \gamma^*) - 2\rho(\alpha_i c_i^2 \gamma_i^* - \alpha_j c_j^2 \gamma_j^*)\theta^* + \rho(\alpha_i^2 c_i^2 \gamma^{*2} - \alpha_j^2 c_j^2 \gamma^{*2})\theta^{*2} + 2\rho(C_{\gamma i} - C_{\gamma j})\theta\left(1 - \ln\left(\frac{\theta}{\theta^*}\right)\right) - 2(\tilde{k}_i - \tilde{k}_j)\theta\Big).$$

The other case $c_i = c_j$ produces the single root

$$\tilde{\gamma}_{i,j}(\theta) = \frac{2(\hat{b}_i - \hat{b}_j) + \rho c^2(\gamma_i^{*2} - \gamma_j^{*2}) - 2(\tilde{k}_i - \tilde{k}_j)\theta}{2\rho c^2(\gamma_i^* - \gamma_j^* + (\alpha_i - \alpha_j)(\theta - \theta^*))} + \tag{3.71}$$

$$\frac{2\rho(C_{\gamma i} - C_{\gamma j})\theta\left(1 - \ln\left(\frac{\theta}{\theta^*}\right)\right) - 2\rho c^2(\alpha_i \gamma_i^* - \alpha_j \gamma_j^*)\theta^* + \rho c^2(\alpha_i^2 \gamma_i^{*2} - \alpha_j^2 \gamma_j^{*2})\theta^{*2}}{2\rho c^2(\gamma_i^* - \gamma_i^* + (\alpha_i - \alpha_j)(\theta - \theta^*))}.$$

For future reference we define phase-1, index i=1 in equation (3.69), as the *parent* phase. The material model will now be restricted such that phase-1 has a free energy that is symmetric with respect to the strain for a fixed temperature. Formally, this assumption is stated:

(A.3) Phase-1, the parent phase, has a free energy $\tilde{\psi}_1$ which is symmetric with respect to the strain γ at fixed temperature θ.

Satisfaction of assumption (A.3) gives

$$\gamma_1^* + \alpha_1(\theta - \theta^*) = 0. \tag{3.72}$$

Since the temperature θ may vary, this requires that $\alpha_1 = 0$ and $\gamma_1^* = 0$. Therefore, in the parent phase the coefficient of thermal expansion vanishes and the reference state is strain free. Furthermore, since a zero value for the coefficient of thermal expansion represents a material which has been deemed separable, implying that the mechanical equations of motion decouple from the equations of thermal evolution, the parent phase material response is referred to as separable.

Henceforth it will be assumed that the bar is composed of a two phase material, one being the separable parent phase defined in (A.3), the other phase being the more general material, i.e. of the nonseparable type, also called *fully thermal.* Formally we express this assumption:

(A.4) The number of phases will be restricted to two, which we will call phase-1 and phase-2 (phase-1 being the parent phase).

Together (A.3) and (A.4) state that the bar consists of a two phase solid, the two phase's having different thermomechanical properties. The reference state for the parent phase was defined to be strain free, and for notational convenience the offset strain in phase-2 is designated $\gamma^* \equiv \gamma_2^*$. Figure 3.1 displays the two phase material's free energy functions for constant temperature, as mentioned earlier these two functions can be visualized as distinct potential wells. Each vertex can be thought of as that energy's ground state, since it is the minimum value for that energy. Shown in Figure 3.1 are arrows located at the vertex of each well, these arrows are to indicate that the vertices are not stationary but may change positions depending on the value of the temperature θ.

3.4.1 The ground-state equivalence temperature

We *define* the *ground-state equivalence* temperature as that temperature for which the ψ- value of the free energy vertices, or ground states, have the same value. At all other temperatures the vertices involve different ψ- values, and thus one phase has a free energy ground state whose ψ- value is less than the other. Thus a ground state equivalence temperature separates temperature intervals associated with a natural change in stability of the ground states. To inquire further into this issue we construct the function $\Delta V(\theta)$ which is defined as the difference between the free energy vertex in phase-2 and that in phase-1

$$\Delta V(\theta) \equiv \psi_2\big|_{\text{vertex}} - \psi_1\big|_{\text{vertex}}. \tag{3.73}$$

In phase-2 the free energy vertex is located at $\gamma = \gamma^* + \alpha_2(\theta - \theta^*)$, while in phase-1 it is at $\gamma = 0$, hence $\Delta V(\theta)$ is expressed

$$\Delta V(\theta) = -\frac{\rho c_2^2 \alpha_2^2}{2}(\theta-\theta^*)^2 + \rho\,(C_{\gamma 2}-C_{\gamma 1})\,\theta\left[1-\ln\left(\frac{\theta}{\theta^*}\right)\right] \tag{3.74}$$

$$-\left(\rho c_2^2\alpha_2\gamma^* + \tilde{k}_2 - \tilde{k}_1\right)\theta + \frac{\rho c_2^2(\alpha_2\theta^*)^2}{2} + \hat{b}_2 - \hat{b}_1 .$$

From the freedom inherent in selecting the normalization temperature θ^* (3.18), the normalization temperature is now *chosen* as the ground-state equivalence temperature. This choice of θ^* requires that $\Delta V(\theta^*) \equiv 0$, which in turn provides a quadratic equation that θ^* must satisfy

$$\theta^{*2} + \frac{2}{\rho c_2^2\alpha_2^2}\left(\rho\,(C_{\gamma 2}-C_{\gamma 1}) - \rho c_2^2\alpha_2\gamma^* - \tilde{k}_2 + \tilde{k}_1\right)\theta^* + \frac{2}{\rho c_2^2\alpha_2^2}(\hat{b}_2 - \hat{b}_1) = 0. \tag{3.75}$$

Since, in general, there are two roots for equation (3.75), there exists two ground-state equivalence temperatures. Solving (3.75) for θ^* yields

$$\theta^* = \frac{-1}{\rho c_2^2\alpha_2^2}\left(\rho\,(C_{\gamma 2}-C_{\gamma 1}) - \rho c_2^2\alpha_2\gamma^* - \tilde{k}_2 + \tilde{k}_1\right) \pm \Theta^*, \tag{3.76}$$

where

$$\Theta^* = \frac{1}{\rho c_2^2\alpha_2^2}\left(\left(\rho\,(C_{\gamma 2}-C_{\gamma 1}) - \rho c_2^2\alpha_2\gamma^* - \tilde{k}_2 + \tilde{k}_1\right)^2 - 2\rho c_2^2\alpha_2^2(\hat{b}_2 - \hat{b}_1)\right)^{\frac{1}{2}}.$$

The model naturally gives rise to phase transformations provided that Θ^* is a real quantity and we henceforth only consider parameter values for which this is the case. For convenience, the two ground-state equivalence temperatures are distinguished from one another based on their relative values, i.e. $\theta_1^* < \theta_2^*$. This ordering depends on the relative values of the material parameters.

From the ordering of the ground-state equivalence temperatures, three distinct temperature intervals naturally arise: $\theta < \theta_1^*$, $\theta_1^* < \theta < \theta_2^*$, and $\theta_2^* < \theta$. One of the phases will have the lower energy ground state in the two intervals $\theta < \theta_1^*$ and $\theta_2^* < \theta$, while the other phase will have the lower energy ground state for the interval $\theta_1^* < \theta < \theta_2^*$. Table 2 summarizes the preferred phase for each of these intervals.

Table 2: Temperature intervals for preferred phase

Temperature interval	Phase with lower energy ground state
$\theta < \theta_1^*$	phase-2
$\theta_1^* < \theta < \theta_2^*$	phase-1
$\theta_2^* < \theta$	phase-2

To verify this table note from an asymptotic analysis of $\Delta V(\theta)$ for $\|\theta - \theta^*\| \gg 0$, that the quadratic component of $\Delta V(\theta)$ is the dominant term. Under such conditions $\Delta V(\theta)$ behaves like a parabola, and the value of this function is either positive or negative depending on the coefficient of the quadratic term, which according to (3.74) is $-\rho c_2^2 \alpha_2^2/2 < 0$. Therefore phase-2 has the lower ground state for temperatures which are much greater or less than both θ_1^* and θ_2^*, which is precisely the two intervals $\theta < \theta_1^*$ and $\theta_2^* < \theta$.

Figure 3.2 schematically shows how the two free energy functions behave for the different temperature intervals. Note that the ground-state equivalence temperature θ_1^* separates a low temperature stable phase-2 material with a shape strain $\gamma^* + \alpha_2(\theta - \theta_1^*)$ from a high temperature stable phase-1 material with no shape strain. This type of material behavior is similar to Austenite/Martensite systems.

It will prove useful for latter purposes to display the ground-state equivalence temperatures for two special cases. The first case being when the specific heats are equal, $C_{\gamma 2} = C_{\gamma 1}$, the ground-state equivalence temperatures (3.76) then simplify to

$$\theta^* = \frac{1}{\rho c_2^2 \alpha_2^2}\left(\rho c_2^2 \alpha_2 \gamma^* + \tilde{k}_2 - \tilde{k}_1\right) \pm \Theta^*, \tag{3.77}$$

$$(C_{\gamma 2} = C_{\gamma 1})$$

$$\Theta^* = \frac{1}{\rho c_2^2 \alpha_2^2}\left(\left(\rho c_2^2 \alpha_2 \gamma^* + \tilde{k}_2 - \tilde{k}_1\right)^2 - 2\rho c_2^2 \alpha_2^2 (\hat{b}_2 - \hat{b}_1)\right)^{\frac{1}{2}}.$$

Note that Θ^* is real if $\hat{b}_2 - \hat{b}_1$ is negative, or if $\hat{b}_2 - \hat{b}_1$ is positive but sufficiently small.

The other case is where both phases are separable and thus $\alpha_2 = 0$. Multiplication of (3.75) by α_2^2 followed by letting $\alpha_2 \to 0$ yields a first order equation for θ^*. Thus one of these two roots θ^* becomes infinite as a result of the singular perturbation. Formally expressing (3.76) in the form

$$\theta^* = \frac{\left(\rho\,(C_{\gamma 2} - C_{\gamma 1}) - \rho c_2^2 \alpha_2 \gamma^* - \tilde{k}_2 + \tilde{k}_1\right)}{\rho c_2^2 \alpha_2^2}\left(-1 \pm \tilde{\Theta}^*\right), \tag{3.78}$$

$$\tilde{\Theta}^* = \left(1 - \frac{2\rho c_2^2 \alpha_2^2 (\hat{b}_2 - \hat{b}_1)}{\left(\rho\,(C_{\gamma 2} - C_{\gamma 1}) - \rho c_2^2 \alpha_2 \gamma^* - \tilde{k}_2 + \tilde{k}_1\right)^2}\right)^{\frac{1}{2}},$$

performing a Taylor series expansion for $\tilde{\Theta}^*$ about $\alpha_2 = 0$, and collecting similar powers of α_2, gives the two different series expansions for θ^*:

$$\theta^* = \frac{2\left[\tilde{k}_2 - \tilde{k}_1 - \rho\,(C_{\gamma 2} - C_{\gamma 1})\right]}{\rho c_2^2 \alpha_2^2} + \frac{2\gamma^*}{\alpha_2} + \frac{\hat{b}_2 - \hat{b}_1}{\rho\,(C_{\gamma 2} - C_{\gamma 1}) - \tilde{k}_2 + \tilde{k}_1} + O(\alpha_2),$$

and

$$\theta^* = -\frac{\hat{b}_2 - \hat{b}_1}{\rho\,(C_{\gamma 2} - C_{\gamma 1}) - \tilde{k}_2 + \tilde{k}_1} + O(\alpha_2).$$

Here, as is standard, $O(z)$ denotes a quantity that, after division by z, is finite as $z \to 0$.

In the limit as $\alpha_2 \to 0$ there are two distinct cases depending on the relative values of material parameters, the results are

$$\left.\begin{aligned} \theta_1^* &= -\infty \\ \theta_2^* &= -\frac{\hat{b}_2 - \hat{b}_1}{\rho\,(C_{\gamma 2} - C_{\gamma 1}) - \tilde{k}_2 + \tilde{k}_1} \end{aligned}\right\} \quad \text{if } \rho\,(C_{\gamma 2} - C_{\gamma 1}) > \tilde{k}_2 - \tilde{k}_1,$$

$$(\alpha_2 = 0) \tag{3.79}$$

$$\left.\begin{aligned} \theta_1^* &= -\frac{\hat{b}_2 - \hat{b}_1}{\rho\,(C_{\gamma 2} - C_{\gamma 1}) - \tilde{k}_2 + \tilde{k}_1} \\ \theta_2^* &= \infty \end{aligned}\right\} \quad \text{if } \rho\,(C_{\gamma 2} - C_{\gamma 1}) < \tilde{k}_2 - \tilde{k}_1.$$

Application of this result would in general restrict attention to a limited temperature range, and the material parameters entering the model would then be chosen as the basis of this temperature range. In particular, temperatures θ are regarded as positive on some absolute temperature scale. However in this section, and from time to time in what follows, it is convenient to treat θ as an arbitrary real number purely for the purpose of clarifying the global mathematical structure of a physical description that would certainly be localized in an application setting. This is the sense in which results like $\theta_1^* = -\infty$ should be considered.

3.4.2 The Latent Heat

Any heat produced or absorbed from the transformation between two equilibrated phases is the latent heat of transformation λ_T. The latent heat of transformation from phase-2 to phase-1 is expressed

$$\lambda_T = \frac{\theta^*}{\rho}\left[\tilde{\eta}_2(\gamma^*, \theta^*) - \tilde{\eta}_1(0, \theta^*)\right]. \tag{3.80}$$

In particular for $\theta^* > 0$, $\rho > 0$ it follows that the transformation from phase-2 to phase-1 is exothermic if $\lambda_T > 0$ and is endothermic if $\lambda_T < 0$.

From definition (3.80) and the existence of two ground-state equivalence temperatures we conclude the existence of two latent heats, one for each ground-state equivalence temperature. The general expression for the latent heat can be computed from (3.19)

$$\lambda_T = \frac{\theta^*}{\rho}\left[\rho c_2^2 \alpha_2 \gamma^* + \tilde{k}_2 - \tilde{k}_1\right] ,$$

which motivates the definition λ_{T1} and λ_{T2} where

$$\lambda_{Ti} = \frac{\theta_i^*}{\rho}\left[\rho c_2^2 \alpha_2 \gamma^* + \tilde{k}_2 - \tilde{k}_1\right] \qquad (i = 1, 2) . \tag{3.81}$$

The difference between the two latent heats is

$$\Delta\lambda_T = \lambda_{T2} - \lambda_{T1} = \frac{2\Theta^*}{\rho}\left[\rho c_2^2 \alpha_2 \gamma^* + \tilde{k}_2 - \tilde{k}_1\right],$$

which does not, in general, vanish. Note however, that $\Delta\lambda_T = 0$ when $\Theta^* = 0$ which corresponds to the existence of a single ground-state equivalence temperature. We henceforth use the generic terms θ^* and λ_T, where the specific ground-state equivalence temperature and latent heat is inferred, when necessary, from the appropriate temperature interval under consideration.

3.5 Summary of the Two Phase Material Model

For future reference the free energy, entropy and stress response for both phases are given below in terms of the more familiar thermodynamic variables, these relationships between the different forms having just been developed. These forms will utilized throughout the remainder of this document.

Phase-2 material:

$$\tilde{\psi}_2(\gamma,\theta) = \frac{\rho c_2^2}{2}\left[\gamma-(\gamma^* + \alpha_2(\theta-\theta^*))\right]^2 + \bar{b}_2\theta\left[1-\ln\left(\frac{\theta}{\theta^*}\right)\right] \tag{3.82}$$

$$-\frac{\rho c_2^2\alpha_2^2}{2}(\theta-\theta^*)^2 - (\rho c_2^2\alpha_2\gamma^* + \tilde{k}_2)\,\theta + \frac{\rho c_2^2(\alpha_2\theta^*)^2}{2} + \hat{b}_2,$$

$$\tilde{\eta}_2(\gamma,\theta) = \bar{b}_2\ln\left(\frac{\theta}{\theta^*}\right) + \rho c_2^2\alpha_2\gamma + \tilde{k}_2, \tag{3.83}$$

$$\tilde{\tau}_2(\gamma,\theta) = \rho c_2^2(\gamma-\gamma^*) - \rho c_2^2\alpha_2(\theta-\theta^*). \tag{3.84}$$

Phase-1 material:

$$\tilde{\psi}_1(\gamma,\theta) = \frac{\rho c_1^2}{2}\gamma^2 + \bar{b}_1\theta\left[1-\ln\left(\frac{\theta}{\theta^*}\right)\right] - \tilde{k}_1\theta + \hat{b}_1, \tag{3.85}$$

$$\tilde{\eta}_1(\theta) = \bar{b}_1\ln\left(\frac{\theta}{\theta^*}\right) + \tilde{k}_1, \tag{3.86}$$

$$\tilde{\tau}_1(\gamma) = \rho c_1^2\gamma. \tag{3.87}$$

In the more familiar thermodynamic variables ρ, μ_i, γ^*, θ^*, $C_{\gamma i}$, α_2, λ_T, $\tilde{k}_1$, $\hat{b}_i$ these functions are

Phase-2 material:

$$
\begin{aligned}
\tilde{\psi}_2(\gamma,\theta) &= \frac{\mu_2}{2}\left(\gamma-(\gamma^*+\alpha_2(\theta-\theta^*))\right)^2+\rho C_{\gamma 2}\theta\left[1-\ln\left(\frac{\theta}{\theta^*}\right)\right]-\frac{\mu_2\alpha_2^2}{2}(\theta-\theta^*)^2 \\
&\quad -\left(\tilde{k}_1+\frac{\rho\lambda_T}{\theta^*}\right)\theta+\frac{\mu_2(\alpha_2\theta^*)^2}{2}+\hat{b}_2, \\
\tilde{\eta}_2(\gamma,\theta) &= \rho C_{\gamma 2}\ln\left(\frac{\theta}{\theta^*}\right)+\mu_2\alpha_2(\gamma-\gamma^*)+\frac{\rho\lambda_T}{\theta^*}+\tilde{k}_1, \\
\tilde{\tau}_2(\gamma,\theta) &= \mu_2(\gamma-\gamma^*)-\mu_2\alpha_2(\theta-\theta^*)\ .
\end{aligned} \tag{3.88}
$$

In the Phase-1 material:

$$
\begin{aligned}
\tilde{\psi}_1(\gamma,\theta) &= \frac{\mu_1}{2}\gamma^2+\rho C_{\gamma 1}\theta\left[1-\ln\left(\frac{\theta}{\theta^*}\right)\right]-\tilde{k}_1\theta+\hat{b}_1, \\
\tilde{\eta}_1(\theta) &= \rho C_{\gamma 1}\ln\left(\frac{\theta}{\theta^*}\right)+\tilde{k}_1, \\
\tilde{\tau}_1(\gamma) &= \mu_1\gamma.
\end{aligned} \tag{3.89}
$$

Although we have not as yet defined a phase selection criterion, given some (γ, θ), we now state that the intersection strains $\gamma_I(\theta)$ (3.70)-(3.71) define the upper/lower *limits* of strain that the material can support in a particular phase given a temperature θ. This assumption is based on the principle of energy minimization as was discussed earlier in calculating (3.70)-(3.71).

We now turn our attention to the stress response for the two phase solid and restrict attention to a single intersection strain γ_I. Then from (3.84) and (3.87) one obtains

$$\begin{aligned} \tilde{\tau}_1(\gamma, \theta) &= \rho c_1^2 \gamma \text{ for phase } 1{:}0 < \gamma < \gamma_I, \\ \tilde{\tau}_2(\gamma, \theta) &= \rho c_2^2(\gamma - \gamma^*) - \rho c_2^2 \alpha_2(\theta - \theta^*) \text{ for phase } 2{:}\gamma \geq \gamma_I, \end{aligned} \tag{3.90}$$

The characteristic feature of the stress-strain response (3.90) is that it is not monotonic. For a fixed temperatures the graph of the material's stress strain response appears like Figure 3.3. Figure 3.3 shows for $\tau \in [\tau_m, \tau_M]$ that the strain does not have a unique value. One can imagine a bar composed of such a two phase material and loaded so that the stress $\tau \in [\tau_m, \tau_M]$, from Figure 3.3 we see that the deformation of the bar is not unique, and for such a load the bar can accommodate a variety of different deformed configurations. Thus under a prescribed load $\tau \in [\tau_m, \tau_M]$ one may only state the possible maximum and minimum deformations.

All of the concepts and ideas concerning the thermodynamic model presented thus far draw upon many of the sources reviewed in Chapter 1. For example, Abeyaratane and Knowles (1993a) have presented a model for the free energy similar to that outlined above. Their model is a three phase solid for which one phase is unstable while the other two are stable. Comparing the free energy models presented in this document with that in Abeyaratane and Knowles (1993a), one finds that the functional dependance on the two field quantities of strain γ and temperature θ is similar. Namely for both models the free energy in either phase can be expressed in the potential well form

$$\psi(\gamma,\theta) = A(\gamma - B(\theta))^2 + C(\theta - \theta^*)^2 + D\theta\left(1 - \ln\left(\frac{\theta}{\theta^*}\right)\right) + E\theta + F, \qquad (3.91)$$

where θ^* is the ground-state equivalence temperature and A, C, D, E, F, are constants and $B(\theta)$ is a function. All of these involve various combinations of the material parameters μ, C_γ, α, γ^*, $\hat{b}$, $\hat{k}$[1]. Each phase may have different material parameters A, C, D, E, F and function $B(\theta)$ associated with (3.91). For the model presented in this document, we have assumed a general form for the two phase solid, where the two phases have distinct material parameters μ_i, $C_{\gamma i}$, α_i, $\hat{b}_i$, $\hat{k}_i$. Abeyaratane and Knowles consider a model which is somewhat less general, the material parameters μ_i, $C_{\gamma i}$, α_i are the same for both of their phases, e.g. the isothermal elastic modulus in phase-1 is equal to that in phase-2, $\mu_1 = \mu_2 = \mu$. Table 3 is a list of the various material parameters in phase-1, A-F, for both the model presented in this document and that in Abeyaratane and Knowles. Table 4 is an analogous presentation for phase-2.

---

[1] Recall from that the isothermal elastic modulus and the acoustic wave speed are related through $c_i = \sqrt{\mu_i/\rho}$, and for this comparative analysis we choose to use the form of the free energy which contains the isothermal elastic modulus.

Table 3: Material parameters in phase-1 for $\psi(\gamma, \theta)$.

Parameter	Abeyaratne and Knowles	$(3.88)_1$
A	$\frac{\mu}{2}$	$\frac{\mu_1}{2}$
$B(\theta)$	$\alpha(\theta - \theta^*)$	0
C	$-\frac{\mu\alpha^2}{2}$	0
D	ρC_γ	$\rho C_{\gamma 1}$
E	0	$-\tilde{k}_1$
F	0	$\hat{b}_1$

From Table 3 we note that, besides $\mu_1 \neq \mu_2$ as mentioned above, the difference in the function $B(\theta)$ and the parameter C stems from assumption A.3, i.e having chosen phase-1 to have a separable form: $\alpha_1 = 0$. The difference in the parameters E and F arises because we have not assumed that the value of the free energy in phase-1 is null at the transformation point (γ^*, θ^*).

Table 4: Material parameters in phase-2 for $\psi(\gamma, \theta)$.

Parameter	Abeyaratne and Knowles	$(3.76)_1$
A	$\frac{\mu}{2}$	$\frac{\mu_2}{2}$
$B(\theta)$	$\gamma^* + \alpha(\theta - \theta^*)$	$\gamma^* + \alpha_2(\theta - \theta^*)$
C	$-\frac{\mu\alpha^2}{2}$	$-\frac{\mu_2\alpha_2^2}{2}$
D	ρC_γ	$\rho C_{\gamma 2}$
E	$\frac{\rho\lambda_T}{\theta^*}$	$-\left(\tilde{k}_1 + \frac{\rho\lambda_T}{\theta^*}\right)$
F	$-\rho\lambda_T$	$\frac{\mu_2(\alpha_2\theta^*)^2}{2} + \hat{b}_2$

We see from Tables 3 and 4 that A, $B(\theta)$, C, and D for both models are essentially the same, the only difference being our assumption that the two phases do not have the same parameters μ, α, C_γ. The constant E and F are somewhat different. Thus we see from this comparison that the model presented in this document is of a similar character to that developed by Abeyaratne and Knowles, however the differences just discussed will play a significant role in the future development.

After developing their model, Abeyaratane and Knowles (1993a) demonstrate its use in a series of numerical simulations for quasi-static processes. The simulations consider the hysteretic response due to stress cycling at constant temperature, temperature cycling at constant stress, and a combination of the two. This same model is used in a later paper, Abeyaratane and Knowles (1993b), where fully dynamical adiabatic motions are considered. They consider a Riemann problem for subsonic phase boundary motion, and they investigate solutions for both a single moving phase boundary and that involving three moving phase boundaries. However, a major simplification in their model is made for the dynamical analysis, namely the coefficient of thermal expansion is assumed to vanish. This assumption, corresponding to a separable material, greatly reduces the complexity of the model and reduces its ability in capturing many thermal effects by limiting all coupling between the temperature and mechanical fields to the jump conditions.

The work presented in this document has the effect of extending that of Abeyaratane and Knowles in a number of directions. We do not make the assumption that both phases possess the same material parameters. Moreover, we investigate the problem for which the primary concern is the analysis of effects when the thermomechanical coupling constant α_2 is a finite quantity. In so doing we clarify the relation between the purely mechanical description and the fully thermomechanical description, especially as regards the dynamics and kinetics of phase boundary motion.

To make this explicit, it will be convenient to introduce a two part decomposition of the field variables into a component which is completely independent of α_2 and a second term which is the α_2 correction. Thus for the generic field variable f the two part decomposition is defined

$$f = f^{o} + f^{\alpha_2}, \tag{3.92}$$

where

$$f^{o} = \lim_{\alpha_2 \to 0} f, \tag{3.93}$$

$$f^{\alpha_2} \equiv f - f^{o} . \tag{3.94}$$

In general, f is a function representing the fully coupled material, which collapses to f^{o} when considering a separable material. The function f^{α_2} is seen to provide the bridge between these two materials. It is to be emphasized that this so far generic function f could represent quantities that are known a-priori, such as the free energy function. Alternatively f could represent quantities that are determined as part of the solution to a problem, such as the field variables (γ, v, θ) that describe physical processes. In the latter case, an exact determination of the function may not be possible in a fully coupled material, but the exact determination may be possible in the reduced problem involving a separable material. In such cases f is unobtainable, whereas f^{o} is obtainable. This, in turn, renders f^{α_2} unobtainable. In such instances it will be extremely useful to understand the leading order effects of thermomechanical coupling by investigating f^{α_2} in the small α_2-limit. In such instances, the perturbation expansion for f^{α_2} becomes a natural object of study.

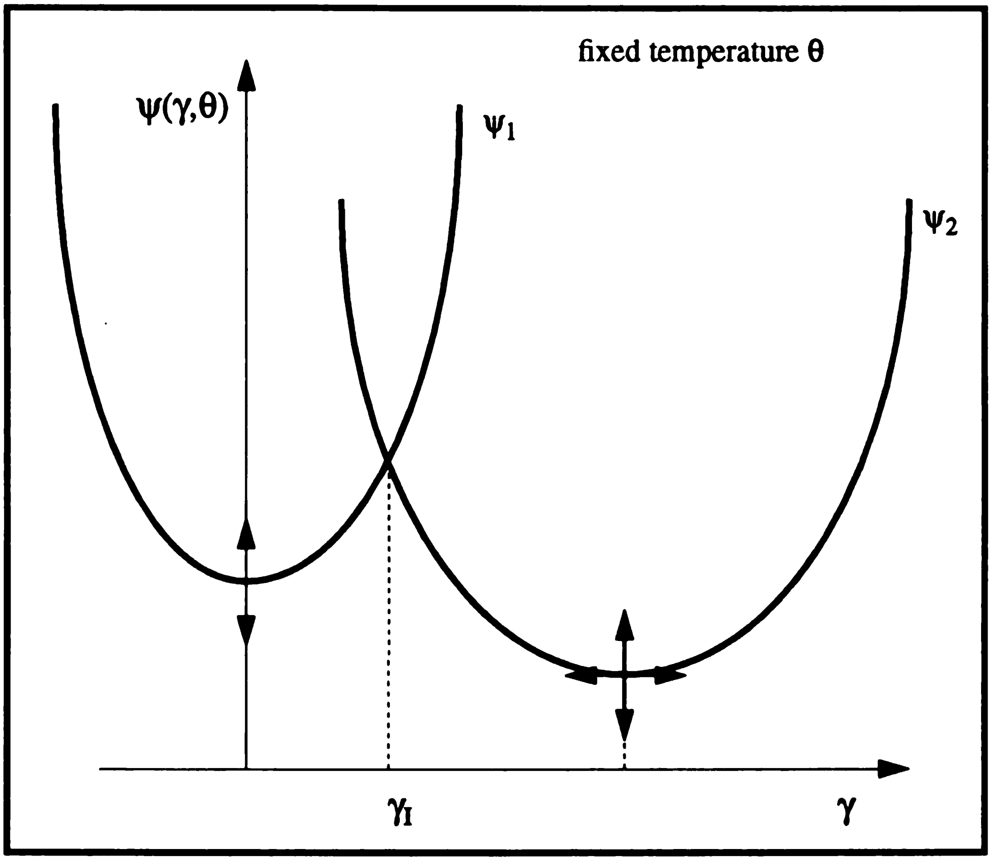

Figure 3.1 This figure is a schematic representation of the Helmholtz free energy function $\psi(\gamma, \theta)$ plotted against the strain γ at a constant temperature θ. Shown are the two free energy functions ψ_1 and ψ_2, each represents a distinct phase of the material.The arrows, which are shown at each of the vertices, acknowledge that the location of these vertices shift as the temperature changes. At each temperature there exists a level of strain for which the values of the free energies are equivalent, this strain is designated γ_I

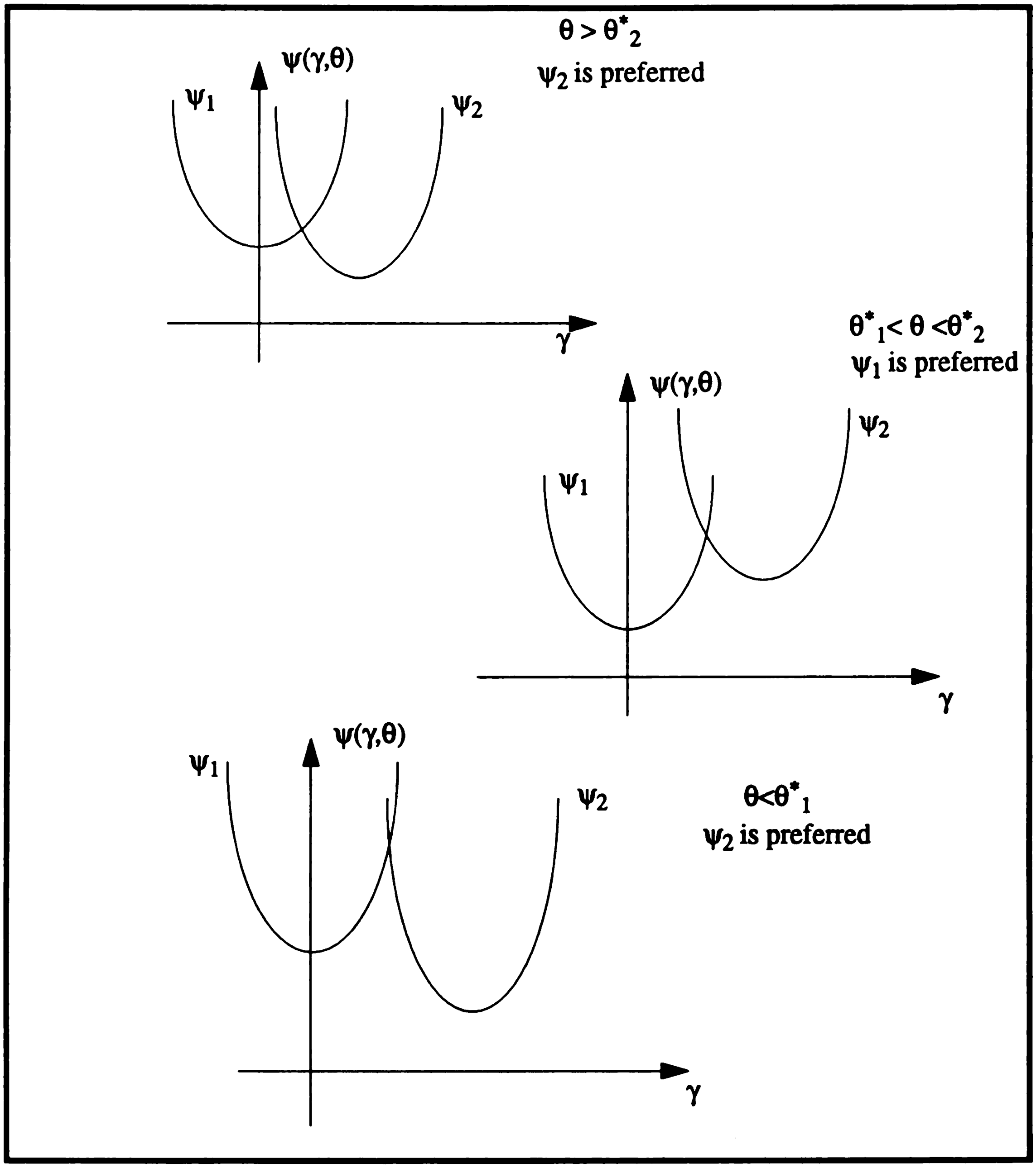

Figure 3.2 This schematically shows how the two free energy functions interrelate for the three temperature intervals. In the intervals $\theta < \theta_1^*$ and $\theta > \theta_2^*$ the phase-2 free energy has a lower vertex and in this sense is the preferred phase. For the interval $\theta_1^* < \theta < \theta_2^*$ phase-1 is the preferred interval.

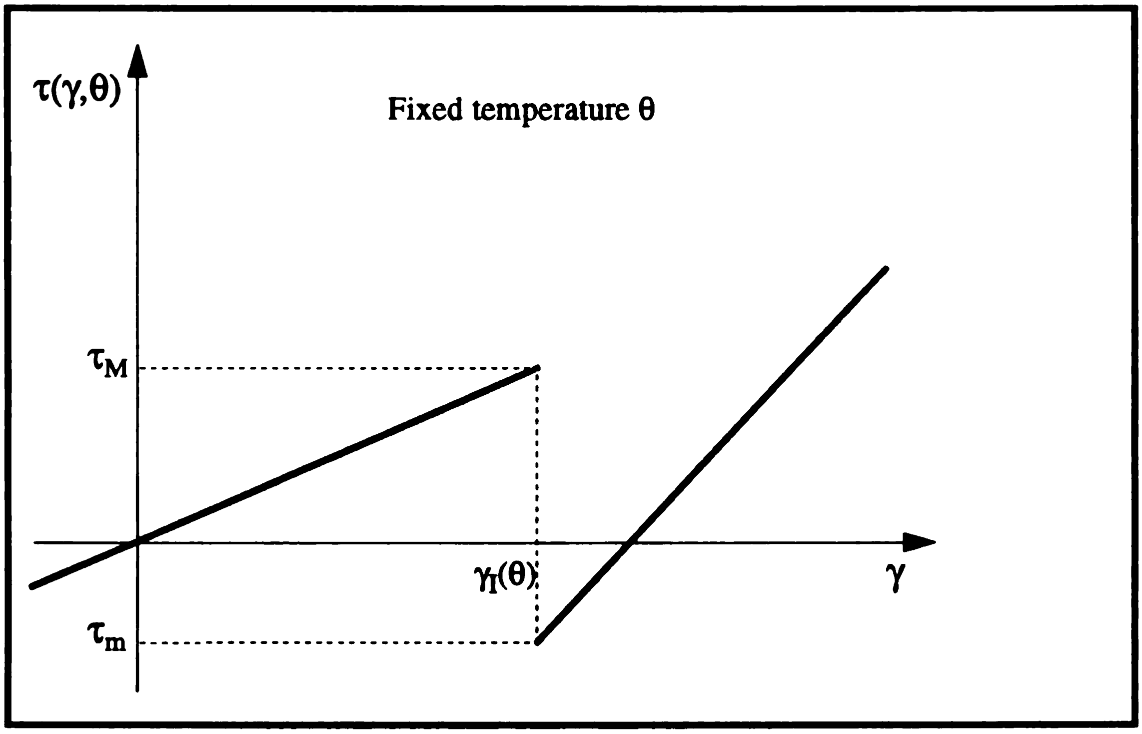

Figure 3.3 The stress-strain response for fixed temperature for the two phase material considered in this document. Both phases have a linear stress strain response, but the overall stress strain response is non-monotonic. From this figure one observes that the strain is not unique for a prescribed stress $\tau \in [\tau_m, \tau_M]$, and thus the bar can accommodate a multitude of different deformed configurations.

4. The Initial Boundary Value Problem

Thus far we have derived a specific constitutive model for a two phase solid, and stated a set of assumptions which we wish to work under. Certain features of the model were then analyzed in order to gain insight into its nature. In this section of the document we define a specific initial boundary value problem for the material with this two-phase constitutive response. The problem to be described is similar to the one considered by Pence (1991a, 1991b), who investigated a purely mechanical problem involving a set of two equations for the two unknown field quantities γ and v, the temperature field being of no concern to that investigation. However in this thesis the major thrust is the consideration of thermal effects.This motivates a more detailed study of two-phase equilibrium initial conditions, which becomes a major focus of this chapter (Section 4.4). A wave pulse is then introduced into this system by imposing an end displacement (Section 4.5). In later chapters we explore the interaction of the pulse with the phase boundary.

4.1 Governing Equations

To begin we state the governing equations of motion for the body in each of the two phases:

$$\frac{\partial \gamma}{\partial t} = \frac{\partial v}{\partial x} \tag{4.1}$$

$$\frac{\partial v}{\partial t} = c_i^2\frac{\partial \gamma}{\partial x} - c_i^2\alpha_i\frac{\partial \theta}{\partial x} \tag{4.2}$$

$$c_i^2\left[\gamma - (\gamma_i^* - \alpha_i\theta^*)\right]\frac{\partial \gamma}{\partial t} + C_{\gamma i}\frac{\partial \theta}{\partial t} = c_i^2\left[(\gamma - \gamma_i^*) - \alpha_i(\theta - \theta^*)\right]\frac{\partial v}{\partial x} \tag{4.3}$$

$$\frac{C_{\gamma i}}{\theta}\frac{\partial \theta}{\partial t} + c_i^2\alpha_i\frac{\partial \gamma}{\partial t} \geq 0 \tag{4.4}$$

where i=1 or 2 and in the parent phase $\alpha_1 = 0$ and $\gamma_1^* = 0$, and in the second phase $\alpha_2 \neq 0$ and $\gamma^* = \gamma_2^*$. The set of equations (4.1)-(4.3) for the unknown field variables γ, v, θ is a system of quasi-linear partial differential equations, and in general is hyperbolic in nature. It is well known that hyperbolic systems with initially smooth fields may at later times break into solutions that are discontinuous (Lax (1973), Renardy and Rogers (1992)). Thus given a set of smooth initial conditions the system (4.1) - (4.3) may admit a solution for the (γ, v, θ) fields which is discontinuous at later times. Here a set of initial/boundary data will proposed and the subsequent initial boundary value problem will be investigated. If solutions can be determined then inequality (4.4) is used to certify admissibility which may either eliminate or place restrictions on the range of the solutions.

4.2 Initial Configurations

Attention is restricted to an initial state with uniform temperature $\hat{\theta}$ that contains a *single* phase boundary, the initial fields $\gamma(x, 0)$, $v(x, 0)$ are taken to be piecewise homogeneous. The initial position of the phase boundary is designated to be s_0. In the initial configuration the material to the left of the phase boundary $(0 < x < s_0)$ is in phase-1, and the material to the right of the phase boundary $(s_0 < x < L)$ is in phase-2.

For the two phases the constitutive response is not the same, and thus they have different sets of governing equations; the significant difference is that the coefficient of thermal expansion α_1 vanishes in phase-1, which decouples the mechanical evolution of the fields from the thermal evolution. Mathematically the two distinct phases will interact across the phase boundary through the Rankine-Hugoniot equations (2.7). In what is to follow the initial temperature and displacement field within the bar are prescribed, this type of initial boundary data is referred to as a hard device.

4.3 Static Configurations

Consider the initial configuration where the strain, velocity and temperature are prescribed. We define an initial configuration to be a *static* configuration if the initial velocity everywhere within the bar vanishes and if the initial temperature field is constant throughout the bar. Thus an initial piecewise-homogeneous configuration that is static and contains a single phase boundary is summarized by

$$\gamma(x,0) = \gamma_o(x) = \begin{cases} \gamma_1 & 0 < x < s_o, \\ \gamma_2 & s_o < x < L, \end{cases} \tag{4.5}$$

$$\begin{aligned} v(x,0) &= 0, \\ \theta(x,0) &= \hat{\theta}. \end{aligned} \tag{4.6}$$

For a single phase boundary to exist it is required that the strains γ_1 and γ_2 satisfy $\gamma_1 < \gamma_I$ and $\gamma_2 > \gamma_I$, where $\gamma_I = \gamma_I(\theta)$ is the intersection strain introduced in Section 3.4. The strain field (4.5) is compatible with the displacement boundary conditions

$$\begin{aligned} u(0,t) &= -\delta_o \\ u(L,t) &= 0 \end{aligned} \qquad \text{for } t < 0, \tag{4.7}$$

provided that δ_o is suitably restricted. To obtain this restriction, consider the average strain γ_o

$$\gamma_o \equiv \frac{1}{L}\int_0^L \frac{\partial u}{\partial x} dx = \frac{\delta_o}{L}. \tag{4.8}$$

From (4.5) and (4.7) the initial displacement field is then

$$\begin{aligned} u(x,0) = u_o(x) &= \gamma_1 x + (\gamma_2 - \gamma_1) s_o - \gamma_2 L \quad \text{on } 0 < x < s_o, \\ u_o(x) &= \gamma_2 (x - L) \quad \text{on } s_o < x < L. \end{aligned} \tag{4.9}$$

The initial location of the phase boundary s_o is then, according to $(4.7)_1$, given by

$$s_o = \frac{(\gamma_2 - \gamma_o) L}{(\gamma_2 - \gamma_1)} \quad \text{where } \gamma_1 < \gamma_o < \gamma_2. \tag{4.10}$$

The restriction that the phase boundary is constrained to the interior of the bar, $0 < s_o < L$, requires that the displacement of the left end of the bar, δ_o, satisfy $L\gamma_1 < \delta_o < L\gamma_2$.

In summary, the temperature $\hat{\theta}$ and the displacement δ_o of the left end of the bar are prescribed in a static configuration, while the right end of the bar remains fixed. To ensure that a single phase boundary is present within the bar requires that the initial displacement δ_o be restricted to a range of values $\delta_o \in [L\gamma_1, L\gamma_2]$. In general, for a given $\hat{\theta}$, the values of γ_1 and γ_2 may vary independently (over some range) while still satisfying this criterion. Thus specification of $\hat{\theta}$ may in general be compatible with a *two* parameter family of strains (γ_1, γ_2) for the initial configuration. Clearly the inability to specify the strains (γ_1, γ_2) indicates that the initial location of the phase boundary cannot be determined from $\hat{\theta}$ and δ_o alone.

4.4 Equilibrium Configurations

Within this framework an initial *equilibrium* configuration is an initial static configurations which also satisfies the equations of equilibrium

$$\frac{\partial \tau}{\partial x} = 0 \text{ and } [[\tau]] = 0. \tag{4.11}$$

Recall that the $[[\cdot]]$ notation denotes the jump in the enclosed quantity across the phase boundary. The initial conditions (4.5) and (4.8) can satisfy the additional equilibrium criteria (4.11), but in so doing the possible range of the initial state of strain will be restricted. The initial strains in a static configuration already satisfy requirement $(4.11)_1$, but $(4.11)_2$ generates an additional relationship between the initial strains (γ_1,γ_2) and the temperature

$\hat{\theta}$ in the initial configuration:

$$\rho c_1^2 \gamma_1 = \rho c_2^2(\gamma_2 - \gamma^*) - \rho c_2^2 \alpha_2(\hat{\theta} - \theta^*). \tag{4.12}$$

From (4.12) it is seen that in an initial equilibrium configuration, two of the three quantities in the triplet $(\gamma_1, \gamma_2, \hat{\theta})$ are independent, the third may be explicitly calculated from the requirement of equilibrium (4.12). Alternatively, at any temperature $\hat{\theta}$ there exists a *one* parameter family of strain pairs (γ_1, γ_2) that satisfy (4.12). The set of initial states $(\gamma_1, \gamma_2, \hat{\theta})$ which satisfy the criteria of an equilibrium configuration may be categorized, and in what is to follow three special types of equilibrium configurations are defined for later use in this study.

4.4.1 Maxwellian Configurations

Considering the set of equilibrium states it is natural to inquire what initial states are energy minimal. For a bar which can support more than one phase, Ericksen (1991) investigated the issues of equilibrium, energy minimization, and stability for both the hard and soft loading devices. For the hard device (the problem under consideration here) he demonstrates that minimization of the Helmholtz free energy requires that the bar must be in an equilibrium configuration, i.e. minimization of the free energy dictates that the fields in the bar must satisfy (4.6) and (4.11). Since this process does not define an unique equilibrium state, further investigation into the absolute minimizer amongst all the possible equilibrium candidates lends itself naturally to defining a stable equilibrium state. Requiring that the equilibrium state be the minimizer for the set of equilibrium states, and thus the most stable, defines the so called *Maxwellian* state. Mathematically the definition of the Maxwellian state is an equilibrium configuration which also satisfies the condition

$$[[\psi]] = \langle\langle\tau\rangle\rangle [[\gamma]] \qquad (\mathrm{MX})\,. \tag{4.13}$$

For notational purposes when identifying the Maxwellian state the abbreviation (MX) will be used. To the extent that (4.12) and (4.13) provide two restrictions on the triplet $(\gamma_1, \gamma_2, \hat{\theta})$ one may surmise that a Maxwellian configuration is a one parameter family of initial states. That is if any one of the triplet $(\gamma_1, \gamma_2, \hat{\theta})$ is specified then the remaining two field quantities are determined from (4.12) and (4.13). Thus, at some fixed temperature $\hat{\theta}$ one anticipates that the strains γ_1 and γ_2 (and hence the stress τ) are determined for the Maxwellian state. We shall denote these strains and stresses as γ_1^{MX}, γ_2^{MX} and τ^{MX}.

Interpreting equation (4.13) graphically one observes that, in a Maxwellian configuration, the Maxwell strains are the two strains joined by common tangent line to the free energy as depicted in Figure 4.1. Figure 4.1 shows the graph of the free energy along with the common tangent line which together graphically identifies the location of the two strains.

By definition $(2.9)_1$ and (4.13) an analogous definition of a Maxwellian state is

$$\int_{\gamma_1}^{\gamma_2} \tilde{\tau}(\gamma, \hat{\theta})\, d\gamma = \langle\langle\tau\rangle\rangle [[\gamma]] \qquad (\mathrm{MX})\,, \tag{4.14}$$

from its graphical construction (4.14) is the so called equal area rule. The equal area rule defines the Maxwell stress as that level of stress such that shaded area under the stress-strain curve but above the line $\tau = \tau^{MX}$ is equal to that area below the line $\tau = \tau^{MX}$ but above the stress-strain curve. This is depicted graphically in Figure 4.2.

For the two phase material considered here a short calculation finds that there are two pairs of Maxwell strains if $c_1 \neq c_2$. The double roots occur because, as recalled from Chapter 3, the case $c_1 \neq c_2$ gives rise to two intersection strains (a result of the Helmholtz free energy function being quadratic in strain) and each of these will in general support the tangent line construction. The general results for the Maxwell strains $(c_1 \neq c_2)$ will not be required in what is to follow and thus are not presented.

We will, in what follows, focus particular attention on the case where the acoustic speeds are equal $(c_1 = c_2 = c)$. This simplifies much of the resulting algebra. In this case there is exactly one intersection strain (3.71) and hence a pair of Maxwell strains (one strain for each phase)

$$\gamma_1^{MX}(\hat{\theta}) = \frac{2(\hat{b}_2 - \hat{b}_1) - \dfrac{2\rho\lambda_T\hat{\theta}}{\theta^*} + \rho c^2\alpha_2(2\theta^* - \hat{\theta}) + 2\rho(C_{\gamma 2} - C_{\gamma 1})\left(1 - \ln\left(\dfrac{\hat{\theta}}{\theta^*}\right)\right)\hat{\theta}}{2\rho c^2(\gamma^* + \alpha_2(\hat{\theta} - \theta^*))},$$

$$\gamma_2^{MX}(\hat{\theta}) = \gamma_1^{MX}(\hat{\theta}) + \gamma^* + \alpha_2(\hat{\theta} - \theta^*). \tag{4.15}$$

At this point it is useful to discuss the differences in equilibrium states between two classes of material: a separable material and a fully coupled material. Continuing with the case $c_1 = c_2$, we now carry out the two part decomposition (3.92) for the Maxwell strains. First that part of a Maxwell strain which is independent of α_2 is determined by letting $\alpha_2 \to 0$ in (4.15), this process yields

$$\gamma_1^{MX0}(\hat{\theta}) = \frac{(\hat{b}_2 - \hat{b}_1)}{\rho c^2 \gamma^*} - \frac{(C_{\gamma 2} - C_{\gamma 1})}{c^2 \gamma^*}\left(\left(\frac{\lambda_T}{(C_{\gamma 2} - C_{\gamma 1})\theta^*} - 1\right) + \ln\left(\frac{\hat{\theta}}{\theta^*}\right)\right)\hat{\theta}\,,$$

$$\gamma_2^{MX0}(\hat{\theta}) = \gamma_1^{MX0}(\hat{\theta}) + \gamma^*\,. \tag{4.16}$$

From (4.16) it is interesting to note that, when the MX equilibrium state is specified, the difference in the two strains as $\alpha_2 \to 0$ is just the transformation strain γ^*. Both strains display a complicated logarithmic temperature dependance.

The second part of the two part decomposition (3.92), for the $c_1 = c_2$ case, is to determine the α_2 dependance for the Maxwell strains. Using results (4.15) and (4.16) in (3.93), one finds the expressions for $\gamma_2^{MX^{\alpha_2}}$ and $\gamma_1^{MX^{\alpha_2}}$ are:

$$\gamma_1^{MX\alpha_2}(\hat{\theta}) = \frac{\alpha_2(\hat{\theta} - \theta^*)\left(\rho\hat{\theta}\left(\frac{\lambda_T}{\theta^*} - (C_{\gamma 2} - C_{\gamma 1})\left(1 - \ln\left(\frac{\hat{\theta}}{\theta^*}\right)\right)\right) - (\hat{b}_2 - \hat{b}_1)\right)}{\rho c^2 \gamma^*(\gamma^* + \alpha_2(\hat{\theta} - \theta^*))} + \frac{\alpha_2^2\hat{\theta}(2\theta^* - \hat{\theta})}{2(\gamma^* + \alpha_2(\hat{\theta} - \theta^*))}$$

$$\gamma_2^{MX\alpha_2}(\hat{\theta}) = \gamma_1^{MX\alpha_2}(\hat{\theta}) + \alpha_2(\hat{\theta} - \theta^*) \tag{4.17}$$

The strains (4.17) also show a complicated logarithmic temperature dependance. The difference in these strains is seen to be the value $\alpha_2(\hat{\theta} - \theta^*)$.

For future reference it will also be useful to obtain the Maxwell strains for the $c_1 = c_2$ case with the additional condition that the specific heats of the two phases are equal. Letting $C_{\gamma 1} = C_{\gamma 2} = C_{\gamma}$ in (4.15) leads to

$$\gamma_1^{MX}(\hat{\theta}) = \frac{2(\hat{b}_2 - \hat{b}_1) + 2\rho\left(c^2\alpha_2^2\theta^* - \frac{\lambda_T}{\theta^*}\right)\hat{\theta} - \rho c^2\alpha_2^2\hat{\theta}^2}{2\rho c^2(\gamma^* + \alpha_2(\hat{\theta} - \theta^*))},$$

$$\gamma_2^{MX}(\hat{\theta}) = \gamma_1^{MX}(\hat{\theta}) + \gamma^* + \alpha_2(\hat{\theta} - \theta^*). \tag{4.18}$$

For this special case, the temperature dependance of the strains is no longer logarithmic, in fact the numerator is quadratic while the denominator is linear in the temperature $\hat{\theta}$.

4.4.2 Mechanically Neutral Configurations

The second canonical equilibrium configuration is the mechanically *neutral* state, for notational purposes it will be abbreviated (MN). Along with the condition of equilibrium (4.12), a mechanically neutral state must satisfy the additional requirement

$$[[\varepsilon]] = \langle\langle\tau\rangle\rangle [[\gamma]] \qquad (MN). \tag{4.19}$$

Note from $(2.5)_3$ that this condition must be satisfied for dynamical processes whenever $\dot{s} \neq 0$. However if $\dot{s} = 0$ then (4.19) need not hold, this accounts for the possibility of equilibrium configurations that are not mechanically neutral. One would thus anticipate that an initial state satisfying (4.19) would allow for a relatively smooth transition from the initial configuration into a dynamic state.

From its definition in terms of an additional restriction on the two parameter family of initial equilibrium states, one anticipates that a mechanically neutral state also defines a one parameter family of initial configurations. Namely, by specifying any one of the triplet $(\gamma_1, \gamma_2, \hat{\theta})$ the criteria (4.19) coupled with the conditions of equilibrium should determine the other two. Thus, analogous to a Maxwellian configuration, for an initial equilibrium temperature $\hat{\theta}$ the mechanically neutral criteria (4.19) determines the two strains γ_1 and γ_2.

An alternative definition of a mechanically neutral state, in terms of the free energy and entropy, can be derived via (3.2) and (4.19)

$$[[\psi]] - \langle\langle\tau\rangle\rangle [[\gamma]] + \hat{\theta} [[\eta]] = 0 \qquad (\mathrm{MN})\,. \tag{4.20}$$

If we assume the initial configuration to be mechanically neutral then the triplet $(\gamma_1, \gamma_2, \hat{\theta})$ must satisfy both

$$\begin{gathered} \frac{\rho c_2^2}{2}(\gamma_2 - (\gamma^* - \alpha_2\theta^*))^2 - \frac{\rho c_1^2}{2}\gamma_1^2 + \rho\,(C_{\gamma 2} - C_{\gamma 1})\,\hat{\theta} + \hat{b}_2 - \hat{b}_1 = \\ \frac{1}{2}\Big(\rho c_2^2(\gamma_2 - \gamma^*) - \rho c_2^2\alpha_2(\hat{\theta} - \theta^*) + \rho c_1^2\gamma_1\Big)(\gamma_2 - \gamma_1) \end{gathered} \tag{4.21}$$

and condition (4.12). If the initial temperature $\hat{\theta}$ is specified, then calculating the roots for produces two pairs of roots for the case $c_1 \neq c_2$. Like the MX state, the MN state has two roots because of the quadratic nature of the free energy function and the difference in curvatures $c_1 \neq c_2$. Furthermore, the general results for the MN strains $(c_1 \neq c_2)$ will not be required in what is to follow and thus are not presented.

Turning our attention to the more tractable case of $c_1 = c_2$, we calculate the mechanically neutral strains when the two phases have a common acoustic wave speed, and like the MX case this calculation yields only a single root for both phases

$$\begin{aligned}\gamma_1^{MN}(\hat{\theta}) &= \frac{2(\hat{b}_2-\hat{b}_1)+2\rho(C_{\gamma 2}-C_{\gamma 1})\hat{\theta}+\alpha_2^2\rho c^2\hat{\theta}^2}{2\rho c^2(\gamma^*-\alpha_2\theta^*)},\\ \gamma_2^{MN}(\hat{\theta}) &= \gamma_1^{MN}(\hat{\theta})+\gamma^*+\alpha_2(\hat{\theta}-\theta^*).\end{aligned} \tag{4.22}$$

From (4.22) both MN strains are seen to vary quadratically with the temperature $\hat{\theta}$. It is interesting to note that the difference in these two strains is $\gamma^*+\alpha_2(\hat{\theta}-\theta^*)$, this difference changing linearly with the temperature $\hat{\theta}$.

Continuing with the case $c_1 = c_2$, it will prove useful to determine the two part decomposition (3.92) for the MN strains (4.22). Proceeding with the decomposition, let $\alpha_2 \to 0$ in (4.22) and simplify the resulting expressions to find

$$\begin{aligned}\gamma_1^{MN0}(\hat{\theta}) &= \frac{(\hat{b}_2-\hat{b}_1)+\rho(C_{\gamma 2}-C_{\gamma 1})\hat{\theta}}{\rho c^2\gamma^*},\\ \gamma_2^{MN0}(\hat{\theta}) &= \gamma_1^{MN0}(\hat{\theta})+\gamma^*.\end{aligned} \tag{4.23}$$

As in the MX case (4.16), the difference between the two strains (4.23) is the transformation strain γ^*. Also note that the temperature dependance in both $(4.23)_{1,2}$ is linear.

Continuing with the two part decomposition for the MN strains $(c_1 = c_2)$, that part of the strains which depend on the α_2 coefficient is found by using definition (3.93) with results (4.22) and (4.23). Carrying out this calculation yields

$$\begin{aligned} \gamma_1^{MN\alpha_2}(\hat{\theta}) &= \frac{\alpha_2\theta^*\left[(\hat{b}_2-\hat{b}_1)+\rho\,(C_{\gamma 2}-C_{\gamma 1})\,\hat{\theta}\right]}{\rho c^2\gamma^*(\gamma^*-\alpha_2\theta^*)}+\frac{\alpha_2^2\hat{\theta}^2}{2(\gamma^*-\alpha_2\theta^*)}, \\ \gamma_2^{MN\alpha_2}(\hat{\theta}) &= \gamma_1^{MN\alpha_2}(\hat{\theta})+\alpha_2(\hat{\theta}-\theta^*). \end{aligned} \tag{4.24}$$

It is seen that the difference between these two strains is a quantity which is linearly dependent on the temperature.

Like the Maxwellian case it will also prove useful to calculate the MN strains for the $c_1 = c_2$ case when the specific heats of the two phases are equal. By requiring that $C_{\gamma 1} = C_{\gamma 2} = C_\gamma$ in (4.22) the MN strains simplify into

$$\begin{aligned} \gamma_1^{MN}(\hat{\theta}) &= \frac{2(\hat{b}_2-\hat{b}_1)+\alpha_2^2\rho c^2\hat{\theta}^2}{2\rho c^2(\gamma^*-\alpha_2\theta^*)}, \\ \gamma_2^{MN}(\hat{\theta}) &= \gamma_1^{MN}(\hat{\theta})+\gamma^*+\alpha_2(\hat{\theta}-\theta^*). \end{aligned} \tag{4.25}$$

For this case the MN strains (4.25) are seen to differ by the temperature function $\gamma^*+\alpha_2(\hat{\theta}-\theta^*)$.

4.4.3 Entropically Neutral Configurations

The third type of canonical type of equilibrium states is the *entropically neutral* state, which will be referred to with the abbreviation (EN). An initial equilibrium configuration is defined to be entropically neutral if it satisfies the additional criteria

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$$[[\eta]] = 0 \qquad (\mathrm{EN})\,. \tag{4.26}$$

From (4.26) an entropically neutral configuration requires that $(\gamma_1, \gamma_2, \hat{\theta})$ satisfy

$$\rho C_{\gamma 2} \ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \rho c_2^2 \alpha_2 (\gamma_2 - \gamma^*) + \frac{\rho \lambda_T}{\theta^*} = \rho C_{\gamma 1} \ln\left(\frac{\hat{\theta}}{\theta^*}\right) \tag{4.27}$$

and (4.12).

Like the Maxwellian and mechanically neutral initial configurations, an entropically neutral initial configuration defines a one parameter family of initial states, by specifying any one of the triplet $(\gamma_1, \gamma_2, \hat{\theta})$ the conditions of equilibrium and (4.27) determines the other two. However, unlike the other two canonical equilibrium configurations, for the case $c_1 \neq c_2$ the entropically neutral criterion yields a *single* root for the two strains $(\gamma_1^{EN}(\hat{\theta}), \gamma_2^{EN}(\hat{\theta}))$ for a given initial temperature $\hat{\theta}$.

Once again we consider the simpler case of equal wave speeds $c_1 = c_2$. Under such an assumption (4.27) gives rise to an algebraic equation for which γ_2^{EN} can be determined, this result coupled with the equilibrium equation $(4.11)_2$ allows for the calculation of γ_1^{EN}. The expressions for the entropically neutral strains are:

$$\begin{aligned} \gamma_1^{EN}(\hat{\theta}) &= -\frac{1}{c^2 \alpha_2}\left((C_{\gamma 2} - C_{\gamma 1}) \ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \frac{\lambda_T}{\theta^*} \right) - \alpha_2 (\hat{\theta} - \theta^*), \\ \gamma_2^{EN}(\hat{\theta}) &= \gamma_1^{EN}(\hat{\theta}) + \gamma^* + \alpha_2 (\hat{\theta} - \theta^*). \end{aligned} \tag{4.28}$$

It is interesting to note that these equilibrium strains are of a different α_2 dependency than either the Maxwellian and the mechanically neutral cases. From (4.28) it is seen that the entropically neutral strains are *singular* in the $\alpha_2 \to 0$ limit, whereas for both the mechanically neutral and Maxwellian cases a finite quantity results from the limit process. The EN strains also display a logarithmic dependance on the temperature $\hat{\theta}$, and thus have a complex temperature dependance.

For the entropically neutral configuration the two part decomposition (3.92) yields some interesting results. Still considering the $c_1 = c_2$ case, we first investigate the case of a separable material. Thus let $\alpha_2 \to 0$ in (4.27), and note that this process removes all dependency on the deformation in condition (4.27). Carrying out the details of this limiting process provides a *specific* temperature for the entropically neutral configuration

$$\hat{\theta}^{EN^0} = \theta^* \exp\left(\frac{\lambda_T}{\theta^* (C_{\gamma 1} - C_{\gamma 2})}\right). \tag{4.29}$$

First, note that the temperature $\hat{\theta}^{EN^0}$ depends only on specific values of material parameters, and thus is a constant value. Second, when $\alpha_2 = 0$, the entropically neutral strains are found via the equations of equilibrium, criterion (4.27) plays no part in their determination. Together these strains form a *one* parameter family. Thus for a separable material the entropically neutral case is quite different than either of the other two canonical configurations. Recall that the MN and MX configurations generated a one parameter family of strains based on specifying an initial temperature, whereas for the EN configuration the initial temperature is specified via (4.29), while the accompanying two strains form an one parameter family of solutions.

Continuing with the focus on materials where $c_1 = c_2$, we consider the case when the two phases have identical values for their respective specific heats, then (4.28) simplifies to

$$\begin{aligned} \gamma_1^{EN}(\hat{\theta}) &= -\frac{\lambda_T}{c^2\alpha_2\theta^*} - \alpha_2(\hat{\theta}-\theta^*), \\ \gamma_2^{EN}(\hat{\theta}) &= \gamma_1^{EN}(\hat{\theta}) + \gamma^* + \alpha_2(\hat{\theta}-\theta^*). \end{aligned} \tag{4.30}$$

Under this restriction the strain $\gamma_1^{EN}(\hat{\theta})$ has a linear temperature behavior, while if one inserts $\gamma_1^{EN}(\hat{\theta})$ into $(4.30)_2$ the strain γ_2^{EN} is seen to be the constant value $\gamma_2^{EN} = \gamma^* - \frac{\lambda_T}{c^2\alpha_2\theta^*}$.

4.4.4 Omnibalanced Configurations

All three of the canonical equilibrium states just introduced (MX, MN, EN) are characterized by a set of strains (γ_1, γ_2) once the temperature $\hat{\theta}$ is specified. Thus the initial temperature $\hat{\theta}$ parameterizes three equilibrium states. In addition since (4.13), (4.19) and (4.26) are distinct equations, these special types of equilibrium states will not, in general, coincide. However there may exist special temperatures for which these states do coincide. These special temperatures, if they exist, will be called *omnibalanced* (OB). Here it is significant to note that an omnibalanced initial state implies any two of (4.13), (4.19) and (4.26) which in turn requires satisfaction of the third. Thus at the special omnibalanced temperatures (if they exist) there exist equilibrium states that are simultaneously MX, MN and EN. Finally, an omnibalanced state, being the intersection of two one parameter families, is an *unique* initial state $(\gamma_1, \gamma_2, \hat{\theta})$.

To formulate the equations which define this configuration, recall that the OB state must simultaneously satisfy the conditions for the MX, MN and EN configurations. Thus, one can choose any pair of strains for either phase-1 or phase-2, say MX and MN, and the difference between theses two strains is required to vanish. Such equations define the OB temperature.This process of obtaining an equation for the OB temperature can proceed using six different pairs:$\gamma_1^{MX} = \gamma_1^{MN}$, $\gamma_1^{MX} = \gamma_1^{EN}$, $\gamma_1^{MN} = \gamma_1^{EN}$ plus the three others that are generated under $1 \rightarrow 2$. Once an OB temperature is determined from one of the six equations, the strains $(\gamma_1^{OB}, \gamma_2^{OB})$ can be calculated by inserting this temperature into one of the three equations (MX, MN, EN) for the strains (γ_1, γ_2). When considering the fully thermal material the calculation of the OB state is algebraically intractable due to the fact the temperature is involved in a logarithmic manner in the strains for both the MX and EN configurations. In fact this algebraic problem persists to the case when the acoustic wave speeds are the same for both phases. Figures 4.3 and 4.4 are graphical representations of all three canonical equilibrium strains versus temperature for both phase-1 and phase-2 respectively. These figures demonstrate that for both phases the three strains intersect at two locations, and it is precisely these locations that represent the omnibalanced state.

However there are two specific cases for which this state can be found, the first being when the acoustic wave speeds and the specific heats are identical for both phases, the second case is when the acoustic wave speeds are identical and both materials are separable.

Consider first the case when $c_1 = c_2$ and $C_{\gamma 1} = C_{\gamma 2}$, then one may determine the OB

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the OB state from the strains (4.18), (4.25) and (4.30) and the knowledge that at an OB temperature all three sets of strains must be equivalent. Using this criterion for the calculation we find the OB criterion provides two sets of initial states, this OB configuration is

$$\hat{\theta}^{OB} = \theta^* - \frac{\gamma^*}{\alpha_2} \pm \frac{\tilde{\gamma}^{OB}}{\alpha_2},$$

$$\gamma_2^{OB} = \gamma^* - \frac{\lambda_T}{\alpha_2 c^2 \theta^*}, \tag{4.31}$$

$$\gamma_1^{OB} = \gamma_2^{OB} + \tilde{\gamma}^{OB},$$

where

$$\tilde{\gamma}^{OB} = \frac{\sqrt{\alpha_2\rho\theta^*\left[-2\rho\lambda_T(\gamma^* - \alpha_2\theta^*) + 2\alpha_2\theta^*(\hat{b}_1 - \hat{b}_2) + \alpha_2\theta^*\rho c^2(\gamma^{*2} - \alpha_2^2\theta^{*2})\right]}}{\alpha_2\rho c\theta^*}.$$

From (3.76) and result $(4.31)_1$ we see that there exists two OB temperatures for each of the ground-state equivalence temperatures θ^*. Since, in Chapter 3, it was shown that there exists two ground-state equivalence temperatures θ_1^* and θ_2^*, given by (3.76), this implies the possibility of four OB temperatures.

Consider now the second case, when both phases are a separable material so that $\alpha_2 = 0$ with $c_1 = c_2$. The OB temperature is now the entropically neutral temperature $\hat{\theta}^{EN}$ (4.29), since by definition the OB state must satisfy all criteria which define the three canonical equilibrium configurations. The strains are found using this OB temperature and the expression for either the MX strains (4.16) or the MN strains (4.23), since both MX and M

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and MN criteria must be satisfied. To summarize, this OB state consists of

$$\hat{\theta}^{OBO} = \theta^* \exp\left(\frac{\lambda_T}{\theta^*(C_{\gamma 1} - C_{\gamma 2})}\right),$$

$$\gamma_1^{OBO} = \frac{\hat{b}_2 - \hat{b}_1 + \rho\theta^*(C_{\gamma 2} - C_{\gamma 1})\exp\left(\frac{\lambda_T}{\theta^*(C_{\gamma 1} - C_{\gamma 2})}\right)}{\rho c^2 \gamma^*}, (\alpha_2 = 0) \tag{4.32}$$

$$\gamma_2^{OBO} = \gamma^* + \gamma_1^{OBO}.$$

This case differs from the previous OB results (4.31), because now there exist only two OB temperatures, one for each value of the ground-state equivalence temperatures (3.76).

With result (4.32) we end any further analysis and development of the OB state. However, there remains a number of open issues concerning the canonical equilibrium states. Most notably would be a study of the correspondence between the transformation and OB temperatures, which should include an analysis of any symmetry relationships which might exist between the four OB temperatures and the two ground-state equivalence temperatures. However, the main focus of this research topic concerns dynamical motions and not equilibrium states, and therefore our study of the equilibrium states ends here.

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4.5 Initial Disturbance

So far we have required the bar to be in an initial equilibrium configuration containing a single phase boundary at s_0. A special set of boundary conditions will now be introduced such that a wave pulse will emerge from the left boundary $(x = 0)$ and travel into the body so as to eventually reach and interact with the phase boundary. The wave pulse originates in phase-1, the phase in which the energy is separable.

The dynamic boundary conditions to be described are active for the period $0 \leq t \leq T_o$. During this interval the left boundary $(x = 0)$ undergoes a smooth ramp-type displacement to a final value δ_F, while the right boundary $(x = L)$ remains fixed. Furthermore, for all time $t > T_o$ it will be required that the displacement at each end remains fixed. This set of initial and boundary conditions corresponds to controlling the displacement and temperature of the ends of the bar, and are commonly referred to as a hard device.

Mathematically this set of boundary conditions is expressed

$$u(0,t) = \begin{cases} -\delta_o - (\delta_F - \delta_o)\dfrac{t}{T_o} & \text{for } 0 \leq t \leq T_o, \\ -\delta_F & \text{for } t > T_o, \end{cases}, \qquad u(L,t) = 0 \text{ for } t \geq 0. \tag{4.33}$$

From the prescribed displacement field (4.33) the corresponding velocities on the two boundaries during the interval $0 \leq t \leq T_o$ are

$$v(0,t) = \begin{cases} -[\delta_F - \delta_o]/T_o \equiv \Delta v & \text{for} \quad 0 \le t \le T_o \\ 0 & \phantom{\text{for}} \quad t > T_o \end{cases},$$

$$v(L,t) = 0 \text{ for } t \ge 0. \tag{4.34}$$

The conditions described by equations (4.33) and (4.34) are such that during the interval $0 < t \le T_o$ the left boundary $x = 0$ undergoes the ramp deformation $u(0,t)$, while simultaneously the boundary $x = L$ remains fixed. The deformation along the lower boundary generates a wave pulse of width $c_1 T_o$, which subsequently propagates into that part of the bar which is in phase-1.

Turning attention to the entrance of the initial wave pulse into the body, the wave pulse's velocity and strain can be mathematically related to the adjacent equilibrium conditions using the Riemann invariants in phase-1. For the period $0 \le t \le T_o$, equations (3.49) and $(3.50)_2$ must be satisfied between the initial equilibrium state and the dynamic state within the wave pulse. More precisely, equation (3.49) restricts changes in entropy, and states that the temperature within the region occupied by the incoming wave packet remains equal to that in the equilibrium state $\dot{\hat{\theta}}$. The second equation $(3.50)_2$ produces a relationship between the initial equilibrium conditions and the strain and velocity fields in the incoming wave. Writing out this second equation gives:

$$c_1 \gamma_1 = \Delta v + c_1 \gamma_w \quad \text{on } \frac{dx}{dt} = -c_1. \tag{4.35}$$

Here Δv is the velocity and γ_w is the strain carried by the wave pulse, the velocity Δv is define

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defined by (4.34). The strain γ_w can be determined by using (4.35) since the strain γ_1 and the velocity within the wave pulse Δv are prescribed.

For future convenience we define the driving strain increment $\Delta\gamma$ to be:

$$\Delta\gamma \equiv \gamma_w - \gamma_1 , \tag{4.36}$$

from (4.35) and (4.36) we find the relationship between the driving strain increment and prescribed velocity Δv is

$$\Delta\gamma = -\frac{\Delta v}{c_1} . \tag{4.37}$$

Here the driving strain increment $\Delta\gamma$ can be thought of as the forcing input to the initial conditions.

Using a similar analysis as that leading to result (4.35), it can be shown that once the initial wave has passed through a particular point in the bar, that point returns to its equilibrium configuration, and remains in that state until another disturbance occurs.

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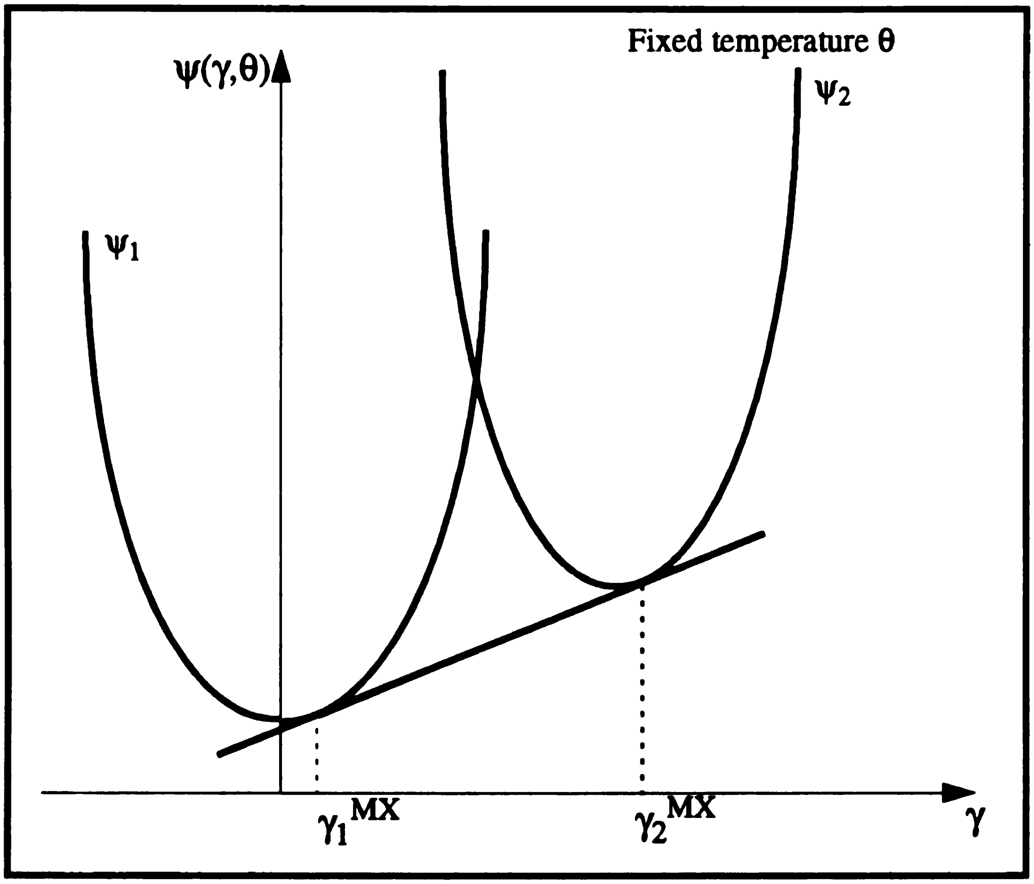

Figure 4.1 This figure is the Helmholtz free energy function $\psi(\gamma, \theta)$ at a constant temperature θ. Shown is one pair of Maxwell strains γ_1^{MX} and γ_2^{MX}. These strains are determined from the requirement that an equilibrium configuration satisfy the criterion $[[\psi]] - \langle\langle\tau\rangle\rangle [[\gamma]] = 0$. Schematically this criterion is shown by the line of slope $\langle\langle\tau\rangle\rangle$ which is tangent to both free energy functions, the points of tangency identify the locations of the Maxwell strains.

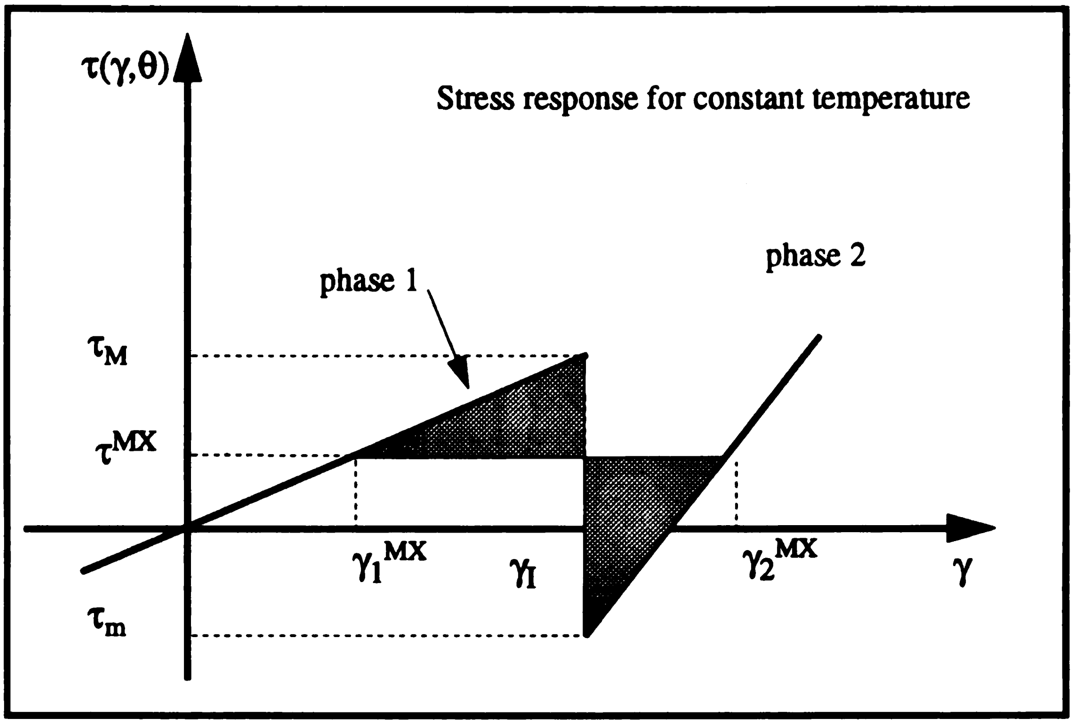

Figure 4.2 Shown is the two phase stress strain response at constant temperature. The Maxwell criterion, $\int_{\gamma_1}^{\gamma_2} \tau(\gamma, \theta)\, d\gamma - \langle\langle\tau\rangle\rangle\, [[\gamma]] = 0$, can be interpreted graphically as the equal area rule. This rule states for the Maxwellian configuration that the area below the phase-1 stress-strain curve but above the line τ^{MX} is equal to the area above the phase-2 stress strain curve but below the line τ^{MX}. On this figure the equal area rule identifies one pair of Maxwell strains γ_1^{MX} and γ_2^{MX}.

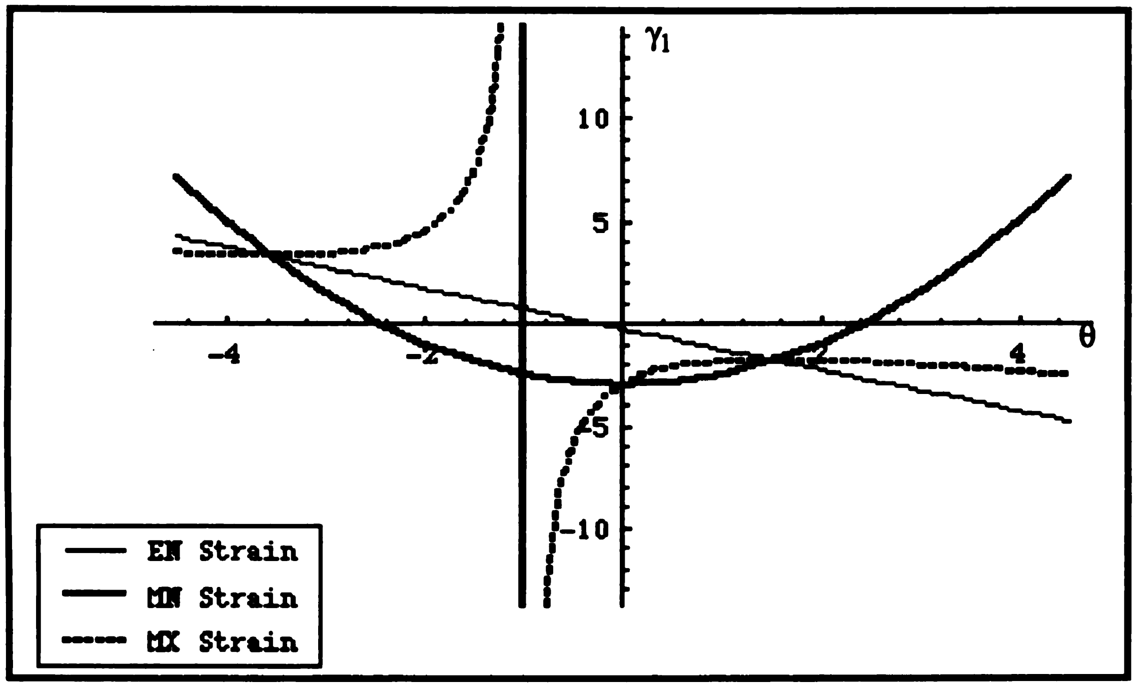

Figure 4.3 This is a schematic representation for the three canonical phase-1 strains for different temperatures. The mutual intersection of all three strains is the location of the omnibalanced temperature $\hat{\theta}^{OB}$. Here the acoustic speeds are the same $c_1 = c_2 = 2$, and the values for the material parameters are $\rho = 1, \theta^* = 1, \gamma^* = 2, C_{\gamma 2} - C_{\gamma 1} = 3,$ $\alpha_2 = 1, \lambda_T = 5.$

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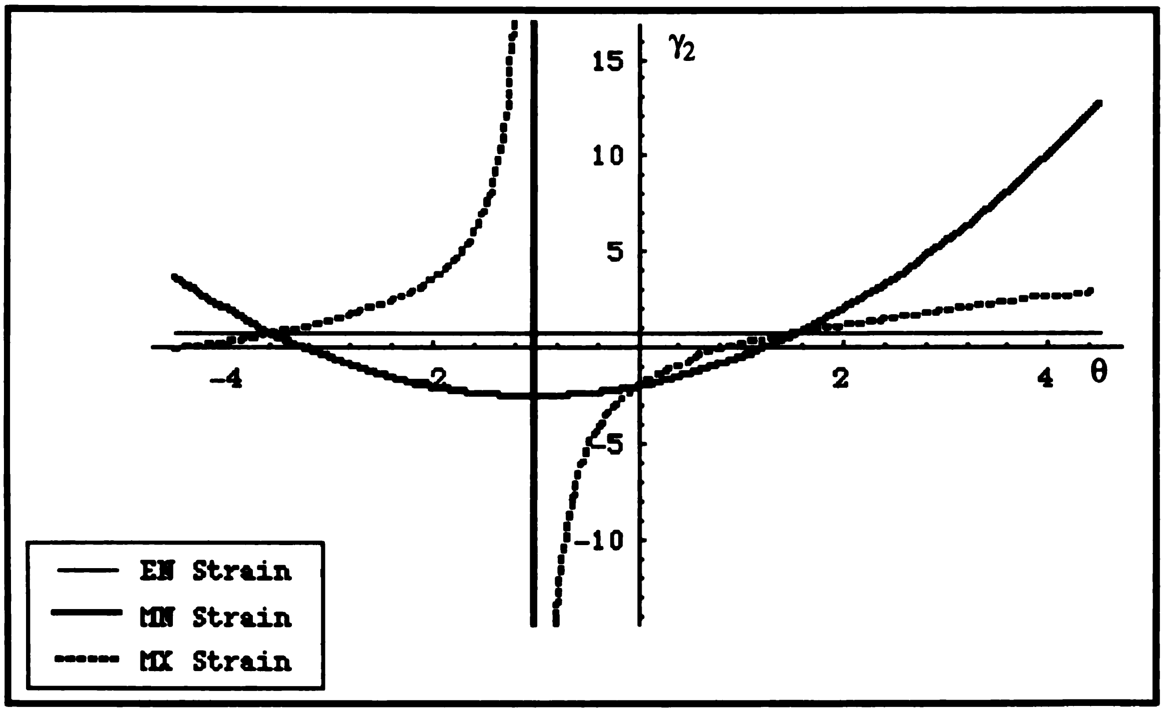

Figure 4.4 This is a schematic representation of the three canonical phase-2 strains for different temperatures. The mutual intersection of all three strains is the location of the omni-balanced temperature $\hat{\theta}^{OB}$. This diagram is the complement of Figure 4.3 in that all the material parameters remain the same as in that figure.

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5. The Interaction of the Initial Wave Pulse with the Phase Boundary

In Chapter 4 a set of initial and boundary data were described, these conditions generate a wave pulse from the left boundary. The pulse travels at speed c_1 from this boundary into the purely mechanical phase (phase-1). At time $t = s_0/c_1$ the pulse will reach the phase boundary and interact with it in some way. In general, the initial interaction of the wave and the phase boundary will set the phase boundary in motion while giving rise to the possibility of a wave being transmitted into the phase-2 region and a wave being reflected back into the phase-1 region. The complexity of such a problem may be understood if the reader recalls similar problems occurring in elastic materials involving the reflection and transmission of a wave striking a boundary, and the subsequent generation and interaction of reflected and transmitted waves (Achenbach 1990).

Pence (1991a,1991b) proposed a similar initial boundary value problem in a two phase elastic solid. In his study Pence considered an infinite layer of material which underwent simple shearing motions. Furthermore, the material model Pence studied was purely mechanical in nature and thus did not consider any contributions of thermal effects. Although geometrically a bar undergoing longitudinal deformations is different than shearing within a layer, mathematically the governing equations for the two different problems are identical. Like Pence we assume that the interaction of the wave pulse and the stationary phase boundary will set the phase boundary in motion, and that the phase boundary will come to rest when the encounter is over. In the following subsection we will compare and contrast the problem Pence investigated with the one under study here, so as to clarify the role that thermal effects play in such a problem.The intention is to identify the similarities and differences between the purely mechanical problem and the fully thermal problem to be considered later.

5.1 The Wave Pulse-Phase Boundary Interaction

In order to explore the temperature effects in the fully thermal problem, while trying to keep the problem under consideration here somewhat similar to Pence's, the following assumptions are made:

(A.5) The initial wave pulse is generated before any interaction with the phase boundary.

(A.6) The interaction of the initial wave pulse with a phase boundary will not lead to the creation of additional phase boundaries.

(A.7) The phase boundary will not encounter either of the boundaries $x = 0$ or $x = L$ during the interaction process.

(A.8) During the interaction the phase boundary will move with a constant speed $\dot{s} = \frac{ds}{dt}$.

(A.9) After the interaction the phase boundary comes to rest.

Assumption (A.5) is satisfied if the time period in which the pulse is generated T_o is restricted such that $T_o < s_o/c_1$. Assumption (A.6) requires that the material to left of the phase boundary $(0 < x < s(t))$ always remains in phase-1, while the material to the right of the phase boundary $(s(t) < x < L)$ is in phase-2. It then follows that the strain field must satisfy:

$$\begin{aligned} \gamma(x,t) &< \gamma_I \text{ for } 0<x<s(t), \\ \gamma(x,t) &> \gamma_I \text{ for } s(t)<x<L. \end{aligned} \tag{5.1}$$

Also, from (A.6) the stress fields on either side of the phase boundary are of the form

$$\begin{aligned} \tau &= \rho c_1^2 \gamma \text{ on } 0 < x < s(t), \\ \tau &= \rho c_2^2(\gamma - \gamma^*) - \rho c_2^2 \alpha_2 (\theta - \theta^*) \text{ on } s(t) < x < L. \end{aligned} \tag{5.2}$$

According to assumption (A.6) the strains γ_w and $\Delta\gamma$, given by (4.36) and (4.37), are restricted in their range of values to the intervals $\gamma_w < \gamma_I$ and $\Delta\gamma < \gamma_I - \gamma_1$. We also note for the interaction to end, and thus satisfy (A.9), that the speed of the phase boundary is bounded by the wave speed on either side $\dot{s} < \min(c_1, c_2)$.

5.2 The Purely Mechanical Problem

In Chapter 3 it was demonstrated that the coupled thermoelastic energy will simplify into a separable energy in the limit $\alpha_2 \to 0$ in which case the thermal and mechanical fields uncouple, yielding a purely mechanical problem and an associated thermal problem. The purely mechanical problem is totally independent of all thermal considerations, and within such a theory one can in principal solve for the mechanical field quantities, $\gamma(x, t)$ and $v(x,t)$, without knowledge of the temperature field. However, the converse is not true, in order to determine the temperature field one must have some knowledge of the mechanical field quantities. Thus, one must first solve the purely mechanical problem and then the thermal problem.

Pence (1991a,1991b) investigated problems similar to the one posed above, but within the framework of a purely mechanical setting, so that no thermal effects were considered. At this time we wish to extract certain key results of his work that will prove most useful in comparison with the results to be derived later in the document.

Temperature is not an issue in the purely mechanical setting, so that the independent field variables are γ, v with the stress $\tau = \tilde{\tau}(\gamma)$. The notion of a separable energy as introduced in this work was not employed by Pence. However, under the current thermodynamic framework, one may classify his treatment as arising from the separable energy function, employed here when $\alpha_2 = 0$. This form of the energy function allows the consideration of the purely mechanical problem, without any acknowledgment of the thermal effects.

Starting with a stationary phase boundary separating the two distinct phases, his treatment introduces a similar wave pulse into the system albeit through the high strain phase. In the current investigation the pulse is introduced through the low strain phase, the high strain phase employed in this document has a temperature dependent stress strain law while the low strain phase does not. By introducing the pulse though the low strain phase we will demonstrate how one may easily solve the pulse propagation problem which communicates the pulse to the phase boundary, so that attention can be focused on the interaction occurring at the phase boundary. Therefore, we first modify the problem studied by Pence, where we again consider the purely mechanical problem but now introduce the pulse into the low strain phase of the material. Henceforth, this problem will be dubbed the *purely mechanical problem.*

The purely mechanical problem introduces the pulse through the low-strain phase; the incoming pulse then strikes the stationary phase boundary and generates a transmitted wave and a reflected wave. The reflected wave interacts with the incident wave in an interaction region. It is easily verified that this problem can be treated by following the exact same procedures employed by Pence in his original problem, i.e. the use of Riemann invariants between adjacent regions leads to a system of six equations. Figure 5.1 graphically depicts this situation in the (x,t)-plane. Furthermore, this figure shows the 6 distinct regions which exist during the interaction: the two undisturbed initial equilibrium states, the region in which the wave pulse exists, and the regions S, R and T. Region R occurs at a later time then either S or T and thus decouples from both, reducing the number of regions to five. Mathematically the field variables in these regions must satisfy the Riemann invariants (3.54) and the jump conditions $(2.7)_{1,2}$.Treating the phase boundary speed as a parameter generates a determinate system of linear equations for the field variables. Solving this system of equations one finds the values of strain γ_T^{mech} and velocity v_T^{mech} in the transmitted region to be

$$\gamma_T^{mech} = \gamma_2 + \frac{(c_1^2 - \dot{s}c_1)2\Delta\gamma - \dot{s}c_1(\gamma_1 - \gamma_2)}{(c_1 + c_2)(c_2 - \dot{s})}, \tag{5.3}$$

$$v_T^{mech} = c_1 c_2 \left[\frac{(\dot{s} - c_1)2\Delta\gamma + \dot{s}(\gamma_1 - \gamma_2)}{(c_1 + c_2)(c_2 - \dot{s})} \right]. \tag{5.4}$$

The values of strain γ_S^{mech} and velocity v_S^{mech} in the interaction region are

$$\gamma_S^{mech} = \gamma_1 + \frac{2c_1c_2\Delta\gamma + \dot{s}[2c_1\Delta\gamma - c_2(\gamma_1 - \gamma_2)]}{(c_1 + c_2)(c_1 + \dot{s})}, \tag{5.5}$$

$$v_S^{mech} = \frac{[-2c_1^2\Delta\gamma + \dot{s}(-2c_2\Delta\gamma - c_2(\gamma_1 - \gamma_2))]c_1}{(c_1 + c_2)(c_1 + \dot{s})}. \tag{5.6}$$

Note that the phase boundary velocity $\dot{s}$ is treated as a parameter and is not specified in the above forms, hence the nonuniqueness of solutions mentioned earlier still holds for the slightly different problem just introduced.

The above analysis describes the initial interaction of the wave pulse with the phase boundary. One may extend this problem to consider the case where the resulting reflected and transmitted wave proceed through the material, eventually striking the end boundaries, which in turn generate new reflected waves traveling back into the body. A simi

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similar problem concerning the hierarchy of ringing waves interacting with a phase boundary was considered by Lin and Pence (1993a), within their study they also analyzed the dissipation of energy resulting from a multitude of wave-phase boundary interactions.

As is well known (James (1983)) dynamical motions of this kind may involve changes in the energy contained within the bar. Under a purely mechanical framework the mechanical energy, $E(t)$, is the sum of two distinct components, the kinetic and strain energies. The rate of change in the mechanical energy is found to be

$$\dot{E}(t) = \frac{d}{dt}F(t) - D(t)\,, \tag{5.7}$$

where

$$F(t) = \int_0^t \{\hat{\tau}(\gamma(h,\xi))\,v(h,\xi) - \hat{\tau}(\gamma(0,\xi))\,v(0,\xi)\}\,d\xi\,, \tag{5.8}$$

$$D(t) = \dot{s}(t)\left\{\int_{\gamma(s(t)-,t)}^{\gamma(s(t)+,t)} \hat{\tau}(\gamma)\,d\gamma - \langle\langle\hat{\tau}(\gamma)\rangle\rangle[[\gamma]]\right\}. \tag{5.9}$$

In this purely mechanical setting the function F(t) represents the work being performed on the external boundaries, while the function D(t) represents the rate change of energy due to phase boundary motion. The expression inside the braces of (5.9) is commonly referred to as the *mechanical driving traction* $f(t)^{\mathrm{mech}}$ (viz. Abeyaratne and Knowles (1991)):

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$$f(t)^{\text{mech}} = \int_{\gamma(s(t)-,t)}^{\gamma(s(t)+,t)} \hat{\tau}(\gamma)\,d\gamma - \langle\langle\hat{\tau}(\gamma)\rangle\rangle[[\gamma]]\,. \tag{5.10}$$

As seen from (5.10) the driving traction provides a source of information on the fields adjacent to the phase boundary. From the definition of the mechanical driving traction the expression (5.9) may be expressed

$$D(t) = \dot{s}(t)\,f(t)^{\text{mech}} \tag{5.11}$$

If $\dot{F}(t) = 0$, then the second law of thermodynamics in this purely mechanical setting motivates the requirement $\dot{E} < 0$. This gives the requirement that admissible motions must satisfy $D(t) \geq 0$, which in turn restricts $\dot{s}(t)\,f(t)^{\text{mech}} \geq 0$. Thus in this purely mechanical setting the quantity $D(t)$ represents the *dissipation rate*.

For the initial encounter calculating the dissipation rate via. (5.9) one obtains

$$D = -\frac{\rho}{2\dot{s}}\left[c_2^2(c_2^2-\dot{s}^2)(\gamma_T-\gamma_2)^2 - c_1^2(c_1^2-\dot{s}^2)(\gamma_S-\gamma_1)^2\right] \tag{5.12}$$

$$+\left(\int_{\gamma_1}^{\gamma_2}\hat{\tau}(\gamma)\,d\gamma - \tilde{\tau}(\gamma_2-\gamma_1)\right).$$

Furthermore, when the initial conditions are Maxwellian (4.14), as considered by Pence, the second bracketed term vanishes and (5.12) reduces to

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$$D = -\frac{\rho}{2\dot{s}}\left[c_2^2(c_2^2-\dot{s}^2)(\gamma_T-\gamma_2)^2 - c_1^2(c_1^2-\dot{s}^2)(\gamma_S-\gamma_1)^2\right] \qquad \text{(MX)}. \qquad (5.13)$$

With significant algebraic manipulation, via. the computer program MATHEMATICA, we express the field quantities γ_T and γ_S on the left hand side of (5.13) in terms of the driving strain $\Delta\gamma$, the initial conditions, and the phase boundary speed $\dot{s}$ via. (5.3) and (5.5). These operations give

$$\begin{aligned} -\frac{\rho}{2\dot{s}}\left[c_2^2(c_2^2-\dot{s}^2)(\gamma_T-\gamma_2)^2 - c_1^2(c_1^2-\dot{s}^2)(\gamma_S-\gamma_1)^2\right] &= \\ \frac{\rho\dot{s}c_1^2\Sigma(\Delta\gamma,\dot{s})}{(c_1+c_2)(c_1+\dot{s})(c_2-\dot{s})}&, \end{aligned} \qquad (5.14)$$

where the function $\Sigma(\Delta\gamma,\dot{s})$ is defined

$$\begin{aligned} \Sigma(\Delta\gamma,\dot{s}) \equiv \dot{s}^2 & [2\Delta\gamma((c_1-c_2)\Delta\gamma - c_2(\gamma_1-\gamma_2))] \\ & -\dot{s}\left[2(c_1-c_2)^2\Delta\gamma^2 - 2c_2(c_1-c_2)(\gamma_1-\gamma_2)\Delta\gamma + c_2^2(\gamma_1-\gamma_2)^2\right] \\ & -[2c_1c_2\Delta\gamma((c_1-c_2)\Delta\gamma - c_2(\gamma_1-\gamma_2))]. \end{aligned} \qquad (5.15)$$

This operation allows the dissipation (5.13) to be expressed

$$D = \frac{\rho\dot{s}c_1^2\Sigma(\Delta\gamma,\dot{s})}{(c_1+c_2)(c_1+\dot{s})(c_2-\dot{s})} \qquad \text{(MX)}. \qquad (5.16)$$

Requiring $D \geq 0$ restricts $\dot{s}$ to an interval of values for each $\Delta\gamma$. From (5.16) and the rest

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restriction on the phase boundary speed $\dot{s} < \min(c_1, c_2)$, the requirement $D \geq 0$ implies that

$$\dot{s}\Sigma(\Delta\gamma, \dot{s}) \geq 0 \qquad (MX), \tag{5.17}$$

and thus an analysis of $\dot{s}\Sigma(\Delta\gamma, \dot{s})$ is sufficient to determine the admissible values $\dot{s}$ for given $\Delta\gamma$, that is the *solution region* in the $(\Delta\gamma, \dot{s})$-plane. Following the analysis in Pence, it is seen that along the line $\dot{s} = 0$ and locus of points $\Sigma(\Delta\gamma, \dot{s}) = 0$ the dissipation vanishes, and thus bounds regions in the $(\Delta\gamma, \dot{s})$-plane to one sign. Figure 5.2 is a plot of the admissability region in $(\Delta\gamma, \dot{s})$-plane for the special case where $c_1 = c_2 = c$. Under these conditions the function $\Sigma(\Delta\gamma, \dot{s})$ reduces to

$$\Sigma(\Delta\gamma, \dot{s}) = -2\dot{s}^2 c\Delta\gamma(\gamma_1 - \gamma_2) - \dot{s}c^2(\gamma_1 - \gamma_2)^2 + 2c^3\Delta\gamma(\gamma_1 - \gamma_2), \tag{5.18}$$

which allows the dissipations function (5.16) to be expressed

$$D = \frac{\rho c\dot{s}\left[-2\dot{s}^2 c\Delta\gamma(\gamma_1 - \gamma_2) - \dot{s}c^2(\gamma_1 - \gamma_2)^2 + 2c^3\Delta\gamma(\gamma_1 - \gamma_2)\right]}{2(c^2 - \dot{s}^2)}. \tag{5.19}$$

Figure 5.2 also illustrates curves of constant dissipation, i.e. $D = \text{constant}$. However, the requirement of positive dissipation does not yield a unique solution for the various field quantities, but only reduces the range of possible values for the parameter $\dot{s}$ for given initial conditions. In particular, if $\Delta\gamma > 0$ then $\dot{s}$ is confined to a range of nonpositive values where both the extreme values $\dot{s} = 0$, $\dot{s} = \dot{s}(\Delta\gamma)|_{\min}$ give $D = 0$. Similarly if $\Delta\gamma < 0$ then $\dot{s}$ is confined to a range of nonnegative values where given the boundary values

$\dot{s} = 0, \dot{s} = \dot{s}(\Delta\gamma)|_{max}$ gives $D = 0$.

To find a unique solution for the results (5.3)-(5.6) one must introduce some additional criterion. Pence (1991a, 1991b) uses a variety of different of selection criteria to determine a unique solution. In the first paper this is achieved by enforcing various requirements on the reflectivity versus transmissivity (a phase boundary impedance), while in the later paper motions are determined under the extremum principle that the dissipation, defined in (5.11), is maximized at each instant.

Another method for selecting physically meaningful solutions is the introduction of a *kinetic relation*, this being an additional constitutive relation which relates the speed of the phase boundary to the various field quantities on either side of the phase boundary. This information is typically provided by the driving traction (5.11). In this purely mechanical setting a standard functional form for a kinetic relation is

$$\dot{s} = \mathcal{F}(f^{mech}),$$

where $\mathcal{F}$ is a functional form motivated by the phase boundary kinetics.The simplest form of a kinetic relation is that of a linear kinetic relation, which implies that the phase boundary speed $\dot{s}$ is a linear function of the driving traction f^{mech}. Mathematically this can be expressed as

$$\dot{s} = \kappa f^{mech}, \tag{5.20}$$

where κ is the *phase boundary mobility*, a material parameter that is here assumed to be cons

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constant. Since $D \geq 0$ implies $\kappa(f^{\mathrm{mech}})^2 \geq 0$, via (5.20), this requires that the mobility κ be a nonnegative quantity. In a similar setting to that of Pence (1991a,b), Lin and Pence (1993a) utilize such a linear kinetic relation and are able to construct an implicit relation between the phase boundary speed and the initial conditions. Furthermore, they are able to show for infinitesimal wave pulses that the maximally dissipative solution is equivalent to the linear kinetic relation for one value of the mobility, and that, in general, this maximally dissipative solution is quantitatively similar to the criterion based on the use of a linear kinetic relation.

For the purely mechanical problem, the use of a linear kinetic relation is now proposed. From (5.11) and (5.16) the driving traction during the initial encounter is

$$f(t)^{\mathrm{mech}} = \frac{\rho c_1^2 \Sigma(\Delta\gamma, \dot{s})}{(c_1 + c_2)(c_1 + \dot{s})(c_2 - \dot{s})} \qquad (\mathrm{MX}). \tag{5.21}$$

Equations (5.16) and (5.20) give rise to

$$\dot{s} = \frac{\kappa \rho c_1^2 \Sigma(\Delta\gamma, \dot{s})}{(c_1 + c_2)(c_1 + \dot{s})(c_2 - \dot{s})} \qquad (\mathrm{MX}), \tag{5.22}$$

which in turn provides an implicit expression for the phase boundary speed. Equation (5.22) admits a unique solution $(\Delta\gamma, \dot{s})$ for the initial encounter, i.e. given a set of initial conditions and the mobility κ, one can determine the phase boundary speed $\dot{s}$ via (5.22). If, following Lin and Pence (1991a), one assumes $c_1 = c_2 = c$ then this implicit equatio

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$$\Delta\gamma = \frac{\dot{s}}{\kappa\rho c^2(\gamma_1-\gamma_2)} + \frac{\dot{s}c(\gamma_1-\gamma_2)}{2(c^2-\dot{s}^2)} \qquad (\mathrm{MX}). \tag{5.23}$$

Figure 5.3 is a graph in $(\Delta\gamma, \dot{s})$ -space of the linear kinetic relation (5.20) for a range of mobilities κ. The graph also shows the criterion $D \geq 0$ which describes the region that contains solutions to (5.23).

For the purely mechanical problem, we have shown for the initial interaction of the wave pulse with the phase boundary that a solution exists if the phase boundary is treated as a parameter. Furthermore, the linear kinetic relation singles out a unique solution. At this point we end our discussion of the purely mechanical problem and return to the fully thermal theory we have developed.

5.3 New Features of the Fully Thermomechanical Interaction

We now turn our attention to the initial interaction of the incoming pulse with the phase boundary under the framework of a fully thermomechanical theory. In this setting, the problem increases in complexity from the purely mechanical theory in essentially three ways.

First, at each point in the domain there are three field variables (γ, v, θ) that must be determined, rather than simply the two mechanical field variables (γ, v) ; only in the limit as the coefficient of thermal expansion vanishes does the temperature field decouple from the mechanical fields.

Second, the new family of characteristic directions $\frac{dx}{dt} = 0$ obtained in (3.63), which are essentially particle paths, introduces a new region into the solution. Recall for the mechanical theory that the interaction gives rise to 5 regions: incident wave, incident/reflection interaction zone, transmitted wave, and the undisturbed initial equilibrium states. In particular, a single region will, in general, encompass *both* transformed and untransformed material (interaction zone if $\dot{s} > 0$, transmitted wave if $\dot{s} < 0$). In the thermomechanical theory this single region bifurcates into two regions (untransformed interaction zone, transformed interaction zone if $\dot{s} > 0$; untransformed transmitted wave, transformed transmitted wave if $\dot{s} < 0$).

Third, in the second phase the wave speed associated with Riemann invariant (3.64) is no longer a constant, but instead is a monotonically increasing function of the temperature

$$\frac{dx}{dt} = \mp c_2 \sqrt{1 + \frac{c_2^2 \alpha_2^2 \theta}{C_{\gamma 2}}}.$$

Thus, in phase-2 the interface between two wave regions supporting different temperatures need not be a *contact discontinuity*[1]. In particular, this is the case for the interface between the T-region, arising from a transmitted wave, and the initially equilibrated phase-2 state, henceforth referred to as the T/E_2 interface (Figure 5.1). Besides the contact discontinuity, the two additional possibilities are a classical *shock* and the *centered simple wave fan* (Whitham (1974)). A centered simple wave fan is also known as a rarefaction

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[1] To avoid confusion, we define a contact discontinuity as a discontinuous surface separating same phase regions that travels at one of the characteristic speeds of the material.This definition is commonly used by mathematicians (Smoller (1983) page 334), investigators in gas dynamics would likely call this a Chapman-Jouget wave (Dunn and Fosdick (1988)). In the problem under study here, the wave speed in phase-1 is given by (3.53) and so any interface between the various regions are again contact discontinuities. Across such contact discontinuities the integration of the characteristic equations yields the Riemann invariants, which can be used to help formulate a solution.

wave in gas dynamics. A shock occurs if the characteristic speed associated with the right propagating Riemann invariant is greater in the T-region than that in the phase-2 equilibrium configuration. In view of the temperature dependance of the speed (3.64), the shock occurs if $\theta_T > \hat{\theta}$. The case of a centered simple wave fan, henceforth simply a *fan*, occurs when the characteristic speed associated with the right propagating Riemann invariant is less in the T-region than that in the phase-2 equilibrium configuration. By use of (3.64) the case of a fan occurs when $\theta_T < \hat{\theta}$.

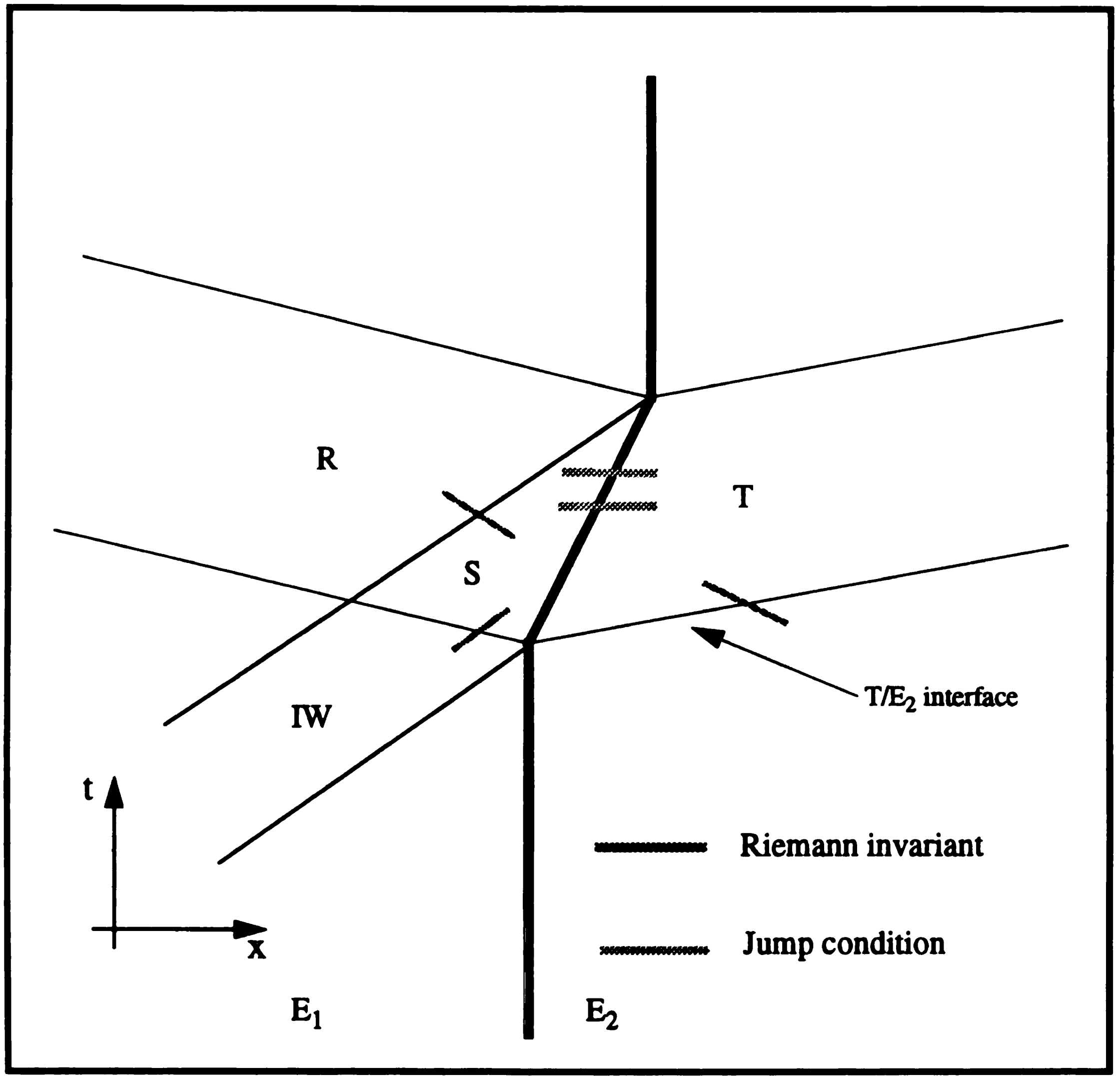

Figure 5.1 This is a graphical representation in the (xt)-plane showing the initial interaction of an incoming pulse with a stationary phase boundary for the purely mechanical problem. The wave speed of the phase boundary is assumed positive $\dot{s}(t) > 0$ in this figure. There exist six distinct regions during this interaction: E_1 & E_2 are the equilibrium configurations in phase-1 and phase-2 respectively, IW represents the region carrying the incoming wave pulse traveling through phase-1, region R is that region in phase-1 where the reflected wave travels, while S arises from the interaction of the incoming wave and the reflected wave; finally region T represents that phase-2 region containing a transmitted wave. The forward movement of the phase boundary transforms phase-2 material into phase-1 material.

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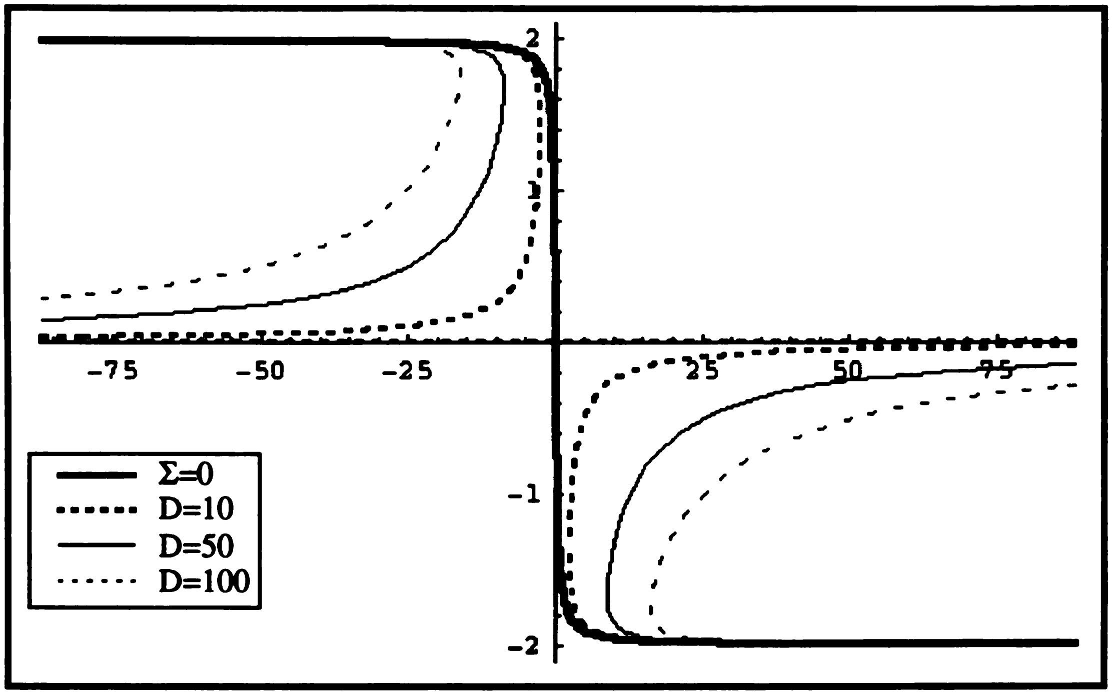

Figure 5.2 This is a schematic representation of the solution region in the $(\Delta\gamma, \dot{s})$-plane for the purely mechanical problem with Maxwellian initial conditions. This region is defined by the criterion of positive dissipation, $D \geq 0$, thus the lines $\Sigma=0$ and $\dot{s} = 0$ provide the boundaries for the admissibility region. Also shown are curves of constant dissipation given by (5.16). The values for the material parameters were chosen to be $c_1 = c_2 = 2, \rho = 1, \gamma_2 - \gamma_1 = 5$.

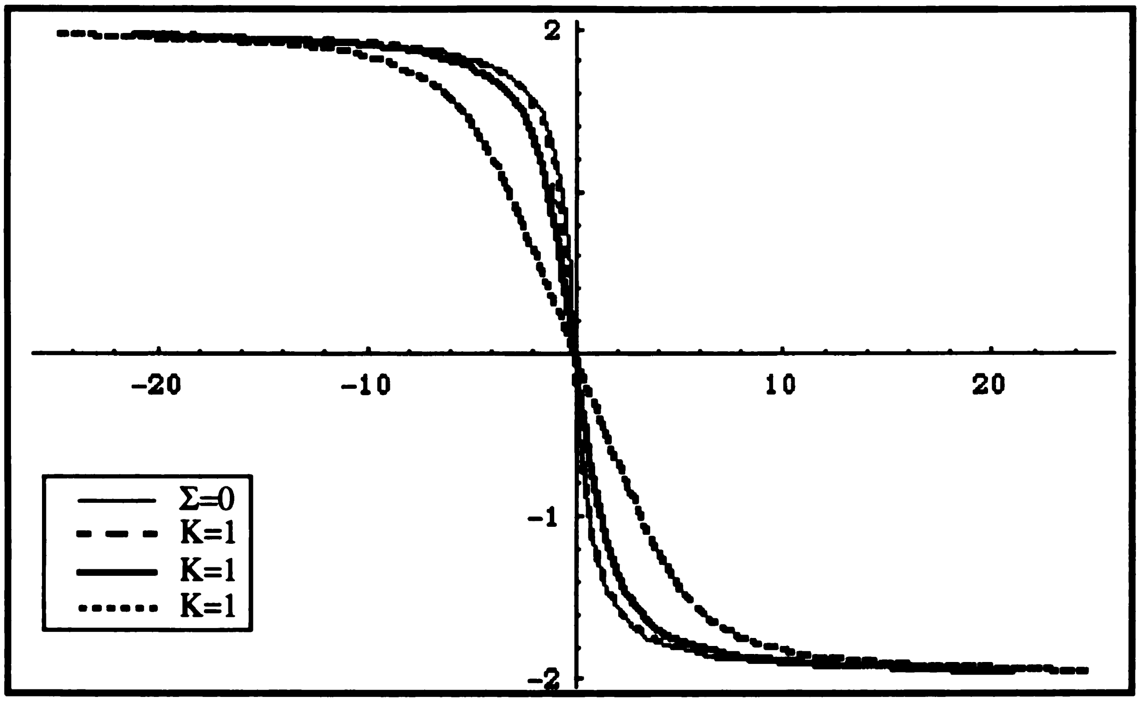

Figure 5.3 This is a schematic representation of the linear kinetic relation with various mobilities κ for the purely mechanical problem with Maxwellian initial conditions. The solid line Σ=0 is the line of zero dissipation ,where Σ is given by (5.18), which divides the plane into regions of positive and negative dissipation. Therefore, under the criterion of positive dissipation, the line Σ=0 also restricts the solution space in the $(\Delta\gamma, \dot{s})$ - plane.The values for the material parameters were chosen to be $c_1 = c_2 = 2, \rho = 1,$ $\gamma_2 - \gamma_1 = 5.$

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6. Analysis of the Initial Interaction Region

6.1 A Method for a Solution to the Initial Boundary Value Problem

The previous development of the characteristic equations and Riemann invariants will now be utilized in an attempt to analyze the changes in the temperature, strain, and stress fields in the proposed initial boundary value problem. Since this method of solution hinges on using the Riemann invariants, any restrictions necessary for the integration of the characteristic equations to produce the Riemann invariants in phase-2 need to be considered.

In view of (A.9) we note that the phase boundary may move with either positive or negative velocity: $\dot{s} > 0$ or $\dot{s} < 0$. For those cases where the phase boundary has negative speeds $\dot{s} < 0$,the characteristic equation (3.60) may no longer be integrated to give the Riemann invariant (3.65). Since it is desired to use the integrated form (3.65) of the characteristic equations to find a solution, the problems investigated are restricted to those for which the phase boundary has a nonnegative value. Recall for the purely mechanical case in which $\alpha_2 = 0$ that this requires that $\Delta\gamma \leq 0$ if the initial state is Maxwellian.

Thus, the $\dot{s} \geq 0$ investigation of the initial interaction consists of two distinct cases: (i) the phase boundary moves with positive velocity $\dot{s} > 0$, and the T/E_2 interface is a fan, and (ii) the phase boundary moves with positive velocity $\dot{s} > 0$, and the T/E_2 interface is a shock. For either case, the characteristic directions and Riemann invariants in phase-1 are given by equations (3.51) and (3.52), while in phase-2 they are given by (3.62) and (3.65). In what is to follow we investigate the case of a fan, with emphasis on how the thermal effects contribute to differences between the purely mechanical theory and the separable and fully thermal theories. The case where the interface is a shock is discussed briefly in Appendix B.

The solution procedure we consider consists of utilizing the jump conditions across the phase boundary along with the Riemann invariants to produce a set of algebraic equations. The field during the initial interaction may be subdivided into five distinct regions centered at $(x, t) = (s_0, s_0/c_1)$. Locally each is wedge shaped. Each region is characterized by a triplet of field values (γ, v, θ). These five regions are given as follows:

IW- The incoming wave in which $(\gamma, v, \theta)_I = (\gamma_1 + \Delta\gamma, -c_1\Delta\gamma, \hat{\theta})$. This region occupies the wedge

$$-\infty < \frac{x - s_0}{t - s_0/c_1} < c_1 .$$

S- The region to the left of the initial position of the phase boundary in which the initial pulse and the wave that has reflected back from the phase boundary are interacting. The triplet values $(\gamma, v, \theta)_S$ are as yet not known. This region occupies the wedge

$$c_1 < \frac{x - s_0}{t - s_0/c_1} < 0 .$$

S^o- The region to the right of the initial position of the phase boundary in which the incoming pulse and the reflected wave are interacting. This region represents the material that changes from phase-2 to phase-1. The triplet of values $(\gamma, v, \theta)_{S^o}$ are as yet not known. The region occupies the wedge

$$0 < \frac{x - s_0}{t - s_0/c_1} < \dot{s}.$$

T- The region in which some part of the initial pulse has transmitted through the phase boundary. The triplet of values $(\gamma, v, \theta)_T$ are also as yet unknown. This region occupies the wedge

$$\dot{s} < \frac{x - s_0}{t - s_0/c_1} < \bar{c}_T \tag{6.1}$$

where the significance of $\bar{c}_T$ is explained below.

E_2- The initial phase-2 equilibrium state in which $(\gamma, v, \theta)_{E_2} = (\gamma_2, 0, \hat{\theta})$. This region occupies the wedge

$$\bar{c}_{E_2} < \frac{x - s_0}{t - s_0/c_1} < \infty.$$

The two velocities $\bar{c}_T$ and $\bar{c}_{E_2}$ that participate in bounding regions T and E_2 are defined as follows. Since we consider the T/E_2 interface to be a centered simple wave fan

$$\bar{c}_T = \sqrt{c_2^2 + \frac{c_2^4 \alpha_2^2 \theta_T}{C_{\gamma 2}}}, \qquad \bar{c}_{E_2} = \sqrt{c_2^2 + \frac{c_2^4 \alpha_2^2 \hat{\theta}}{C_{\gamma 2}}}. \tag{6.2}$$

The existence of a fan region requires that $\dot{c}_T < \dot{c}_{E_2}$ which is equivalent to $\theta_T < \hat{\theta}$. It is to be noted that (6.1) and (6.2) give

$$\dot{s} < c_2\sqrt{1 + \frac{c_2^2\alpha_2\theta_T}{C_{\gamma 2}}}. \qquad (6.3)$$

By use of the Riemann invariants and the Rankine-Hugoniot jump conditions these five regions can be mathematically related to one another, and it is this algebraic dependence that we incorporate. Figure 6.1 is a graphical aid in the assembly of these equations. This figure represents the initial interaction in the xt-plane, shown are regions R, S, S^o and T, the initial wave pulse in the phase-1 region, and the fan in phase-2. This figure also shows the various characteristics and Riemann invariants which link the different regions of the same phase separated by these characteristics, as well as the jump conditions across the phase boundary.

From assumption (A.7) it is required that regions R, S, and S^o are all in phase-1, while T is in phase-2; mathematically these conditions may be expressed as restrictions on the value of various strains

$$\gamma_S < \gamma_I, \qquad \gamma_{S^o} < \gamma_I, \qquad \gamma_I < \gamma_T. \qquad (6.4)$$

Region R, which contains the final reflected wave, occurs later in time than either S, S, or T,^{o} and thus its treatment decouples from these three regions. Thus, the analysis for the initial interaction need only consider the three regions: S, S^o, and T.

Using the method of characteristics one may show that the fields in the regions S, S^o, and T are connected to each other by the following mathematical conditions: across the contact discontinuity between the incoming pulse and S the field variables must satisfy the Riemann invariant conditions (3.51) and $(3.52)_1$, across the contact discontinuity between regions S and S^o the Riemann invariant conditions $(3.52)_{1,2}$, across the moving phase boundary between S^o and T the 3 jump conditions $(2.7)_{1,2,3}$, and across the contact discontinuity between T and the initial phase-2 equilibrium state the Riemann invariant conditions (3.62) and $(3.65)_1$.

The procedure outlined generates a system of nine equations for the nine field quantities: γ_S, v_S, θ_S, γ_{S^o}, v_{S^o}, θ_{S^o}, γ_T, v_T, θ_T and the phase boundary speed $\dot{s}$. Guided by Figure 6.1 and the above outline, the nine equations generated by this process are as listed.

The incoming pulse and region S:

$$-c_1(\gamma_1 + 2\Delta\gamma) = v_S - c_1\gamma_s, \tag{6.5}$$

$$\rho C_{\gamma 1}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \tilde{k}_1 = \rho C_{\gamma 1}\ln\left(\frac{\theta_S}{\theta^*}\right) + \tilde{k}_1. \tag{6.6}$$

Region S and S_0:

$$v_{S^o} - c_1\gamma_{S^o} = v_S - c_1\gamma_S, \tag{6.7}$$

$$v_{S^o} + c_1\gamma_{S^o} = v_S + c_1\gamma_S. \tag{6.8}$$

Region T and the phase-2 equilibrium state:

$$\rho C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \rho c_2^2\alpha_2\gamma_2 + \tilde{k}_2 = \rho C_{\gamma 2}\ln\left(\frac{\theta_T}{\theta^*}\right) + \rho c_2^2\alpha_2\gamma_T + \tilde{k}_2, \tag{6.9}$$

$$\begin{gathered} -\sqrt{C_{\gamma 2}}\left[2\Phi(\hat{\theta}) + \Phi(0)\ln\left(\frac{\Phi(\hat{\theta}) - \Phi(0)}{\Phi(\hat{\theta}) + \Phi(0)}\right)\right] = \\ v_T - \sqrt{C_{\gamma 2}}\left[2\Phi(\theta_T) + \Phi(0)\ln\left(\frac{\Phi(\theta_T) - \Phi(0)}{\Phi(\theta_T) + \Phi(0)}\right)\right], \end{gathered} \tag{6.10}$$

where

$$\Phi(\theta) = \sqrt{\theta + \frac{C_{\gamma 2}}{c_2^2\alpha_2^2}}.$$

Region S_0 and T:

$$-\dot{s}(\gamma_T - \gamma_{S^\circ}) = v_T - v_{S^\circ}, \tag{6.11}$$

$$-\dot{s}\rho(v_T - v_{S^\circ}) = \rho c_2^2(\gamma_T - \gamma^*) - \rho c_2^2\alpha_2(\theta_T - \theta^*) - \rho c_1^2\gamma_{S^\circ}, \tag{6.12}$$

$$\begin{gathered} \left[\frac{1}{2}\rho c_2^2\left(\gamma_T - \left(\gamma^* - \alpha_2\theta^*\right)\right)^2 + \rho C_{\gamma 2}\theta_T + \hat{b}_2\right] - \left[\frac{1}{2}\rho c_1^2\gamma_{S^\circ}^2 + \rho C_{\gamma 1}\theta_{S^\circ} + \hat{b}_1\right] = \\ \frac{1}{2}\left[\rho c_1^2\gamma_{S^\circ} + \rho c_2^2(\gamma_T - \gamma^*) - \rho c_2^2\alpha_2(\theta_T - \theta^*)\right](\gamma_T - \gamma_{S^\circ}). \end{gathered} \tag{6.13}$$

The equations, (6.5) through (6.13), are a system of nine equations for the ten quantities

γ_S, v_S, θ_S, $\gamma_{S\circ}$, $v_{S\circ}$, $\theta_{S\circ}$, γ_T, v_T, θ_T, $\dot{s}$. As it is not clear as to whether a solution for this problem exists, we propose treating $\dot{s}$ as a parameter and investigating the family of solutions resulting from the system of equations and field quantities.

6.2 The Master Equation for the Initial Interaction

By treating the phase boundary speed $\dot{s}$ as a parameter the problem presented by (6.5)-(6.13) reduces to a system of nine equations and nine unknowns. Although a simple algebraic elimination of the various field quantities is not immediate, it can be shown that a laborious elimination process leads to a single master equation for the temperature θ_T which is independent of the other eight unknown field quantities. The other unknown field quantities can then be written in terms of the temperature θ_T and the phase boundary speed $\dot{s}$. Therefore, if a solution to this master equation can be found then we have determined one family of solutions to the system of equations. The reader is directed to Appendix A for a discussion of the actual reduction technique.

The master equation for θ_T is the nonlinear algebraic equation

$$\begin{aligned}&\sqrt{C_{\gamma 2}}\,(c_1-\dot{s})\,\vartheta\,(\theta_T)-\frac{C_{\gamma 2}(\dot{s}c_1-c_2^2)}{c_2^2\alpha_2}\ln\left(\frac{\theta_T}{\theta^*}\right)+c_2^2\alpha_2\theta_T= \\ &\sqrt{C_{\gamma 2}}\,(c_1-\dot{s})\,\vartheta\,(\hat{\theta})-\frac{C_{\gamma 2}(\dot{s}c_1-c_2^2)}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right)+c_2^2\alpha_2\hat{\theta}+(\dot{s}c_1-c_1^2)2\Delta\gamma+\dot{s}c_1\,(\gamma_1-\gamma_2)\,,\end{aligned} \tag{6.14}$$

where

$$\vartheta(\theta) = 2\Phi(\theta) + \Phi(0)\ln\left[\frac{\Phi(\theta) - \Phi(0)}{\Phi(\theta) + \Phi(0)}\right], \qquad (6.15)$$

$$\Phi(\theta) = \sqrt{\theta + \frac{C_{\gamma 2}}{c_2^2\alpha_2^2}}.$$

A closed form solution for this equation is not obvious.

Equation (6.14) may be viewed as an algebraic equation for the temperature θ_T. Values θ_T satisfying this equation will be a function of the incremental forcing strain $\Delta\gamma$ and the phase boundary speed $\dot{s}$. Thus a complete knowledge of the initial and boundary conditions does not provide sufficient information for the determination of a unique temperature θ_T.

Once a value θ_T satisfying (6.14) is obtained, it can be shown that the other eight field quantities $(\gamma_S, v_S, \theta_S, \gamma_{S^\circ}, v_{S^\circ}, \theta_{S^\circ}, \gamma_T, v_T)$ will satisfy the nine governing equations (6.5)-(6.13) if and only if they are given by the following expressions:

$$\gamma_T = \gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right), \qquad (6.16)$$

$$v_T = \sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right], \qquad (6.17)$$

$$\gamma_{S^\circ} = (c_1 + \dot{s})^{-1}\left[\sqrt{C_{\gamma 2}}(\vartheta(\theta_T) - \vartheta(\hat{\theta})) + c_1(\gamma_1 + 2\Delta\gamma) + \dot{s}\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right)\right], \qquad (6.18)$$

$$v_{S^\circ} = \frac{c_1}{\dot{s} + c_1}\left[\sqrt{C_{\gamma 2}}\left(\vartheta(\theta_T) - \vartheta(\hat{\theta})\right) + \dot{s}\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2 \alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right) - \dot{s}\left(\gamma_1 + 2\Delta\gamma\right)\right], \quad (6.19)$$

$$\theta_{S^\circ} = T_1(\theta_T) + T_2(\theta_T) + \left[T_3(\theta_T) + T_4(\theta_T)\right] T_5(\theta_T), \quad (6.20)$$

$$v_S = v_{S^\circ}, \quad (6.21)$$

$$\gamma_S = \gamma_{S^\circ}, \quad (6.22)$$

$$\theta_S = \hat{\theta}. \quad (6.23)$$

The expression (6.20) for θ_{S° makes use of the auxiliary functions:

$$T_1(\theta_T) \equiv \frac{1}{\rho C_{\gamma 1}}\left[\frac{\rho c_2^2}{2}\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2 \alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right) - (\gamma^* - \alpha_2 \theta^*)\right)^2 + \rho C_{\gamma 2}\theta_T + \hat{b}_2 - \hat{b}_1\right],$$

$$T_2(\theta_T) \equiv \frac{-c_1^2}{2C_{\gamma 1}(c_1 + \dot{s})^2}\Bigg(\sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right] + c_1(\gamma_1 + 2\Delta\gamma)$$

$$+ \dot{s}\left[\gamma_2 + \frac{C_{\gamma 2}}{c_2^2 \alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right]\Bigg)^2,$$

$$T_3(\theta_T) \equiv \frac{\rho c_1^2}{(c_1 + \dot{s})}\left[\sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right] + c_1(\gamma_1 + 2\Delta\gamma) + \dot{s}\left[\gamma_2 + \frac{C_{\gamma 2}}{c_2^2 \alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right]\right],$$

$$T_4(\theta_T) \equiv \rho c_2^2\left[\gamma_2 + \frac{C_{\gamma 2}}{c_2^2 \alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right) - (\gamma^* - \alpha_2 \theta^*)\right] - \rho c_2^2 \alpha_2 \theta_T,$$

$$T_5(\theta_T) \equiv \frac{1}{2\rho C_{\gamma 1}(c_1 + \dot{s})}\Bigg(\sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right] + c_1(\dot{s} + 2\Delta\gamma)$$

$$-c_1\left[\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right]\Bigg).$$

From the master equation (6.13) it is seen that $\Delta\gamma$ is a variable which acts as a forcing parameter. For each $\Delta\gamma$, the freedom to vary $\dot{s}$ is anticipated to generate a family of solutions, satisfying all the mathematical balance laws, for each initial-boundary value problem characterized by the forcing parameter $\Delta\gamma$.

For future discussion of the master equation it is convenient to rewrite (6.14) in the form

$$\Psi(\theta_T, \dot{s}, c_1, c_2, C_{\gamma 2}, \theta^*, \alpha_2) - \Psi(\hat{\theta}, \dot{s}, c_1, c_2, C_{\gamma 2}, \theta^*, \alpha_2) \tag{6.24}$$

$$-\omega(\Delta\gamma, \dot{s}, \gamma_1 - \gamma_2, c_1) = 0.$$

This uses the functions

$$\Psi(\hat{\theta}, \dot{s}, c_1, c_2, C_{\gamma 2}, \theta^*, \alpha_2) \equiv \sqrt{C_{\gamma 2}}(c_1 - \dot{s})\,\vartheta(\theta) - \frac{C_{\gamma 2}}{c_2^2\alpha_2}(\dot{s}c_1 - c_2^2)\ln\left(\frac{\theta}{\theta^*}\right) + c_2^2\alpha_2\theta\,,$$

$$\omega(\Delta\gamma, \dot{s}, \gamma_1 - \gamma_2, c_1) \equiv (\dot{s}c_1 - c_1^2)2\Delta\gamma + \dot{s}c_1(\gamma_1 - \gamma_2)\,. \tag{6.25}$$

Since $\omega(0, 0, \gamma_1 - \gamma_2, c_1) = 0$ it follows that $\theta_T = \hat{\theta}$ provides a solution to (6.24) whenever $\Delta\gamma = 0$ and $\dot{s} = 0$. This is simply the persistence of the initial state in the absence of a disturbance $\Delta\gamma$. However, neither $\Delta\gamma = 0$ with $\dot{s} \neq 0$, nor $\dot{s} = 0$ with $\Delta\gamma \neq 0$, gives $\omega = 0$. Thus while $\theta_T = \hat{\theta}$ is a solution of (6.14) when both $\Delta\gamma = 0$ and $\dot{s} = 0$, in general $\theta_T \neq \hat{\theta}$ if either $\Delta\gamma \neq 0$ or $\dot{s} \neq 0$. Solutions θ_T to (6.14) with $\Delta\gamma = 0$ and $\dot{s} \neq 0$ correspond to spontaneous motion of the phase boundary in the absence of an initial disturbance. Solutions θ_T to (6.14) with $\Delta\gamma \neq 0$ and $\dot{s} = 0$ generate dynamical motions with an immobile phase boundary.

Once any solution to the master equation is determined, the strains $\gamma_S, \gamma_{S^\circ}, \gamma_T$ must comply with all restrictions on the transformation of new phases as given in (6.4), which in turn will place restrictions on the range of the initial strain increment $\Delta\gamma$. An explicit solution of (6.14) is not as yet known. However, later in this research we construct a solution for (6.14) under the constraint of $\alpha_2 \ll 1$, for which more quantitative information on the admissibility of $\Delta\gamma$ is presented.

It is interesting to note that (6.24) is satisfied when $\theta_T = \hat{\theta}$ and $\omega = 0$, which corresponds to phase boundary motion in the absence of a transmitted wave. This is seen by letting $\theta_T = \hat{\theta}$ in equations (6.16) and (6.17). For this case the speed of propagation of the phase boundary is determined from the satisfaction of $\omega = 0$

$$\dot{s} = \frac{c_1 2\Delta\gamma}{2\Delta\gamma + (\gamma_1 - \gamma_2)}. \tag{6.26}$$

6.3 Construction of the Centered Simple Wave Fan

Recall that the T/E_2 interface here is a centered simple wave fan, and within this region it is required that the three field quantities γ, v, and θ exist in self-similar form. In order to construct the self-similar solution it is required that the slope $\frac{dx}{dt}$ of the Riemann invariant (3.65) change smoothly from one edge of the fan to the other. Mathematically this condition can be expressed as $\Lambda = \frac{dx}{dt}$, where Λ may vary throughout the fan region. The fan is the wedge shaped region depicted in Figure 6.2, this region being contiguous with the region T and the phase-2 equilibrium configuration. In Figure 6.2 it is shown that at the time t* the two outer edges of the fan are located at $x = x_1$, for which the fan's reciprocal slope is $\Lambda_1 = \frac{dx}{dt}$, and at $x = x_2$ for the reciprocal slope $\Lambda_2 = \frac{dx}{dt}$; the ordering of these quantities being $x_1 < x_2$ and $\Lambda_1 < \Lambda_2$. One may express the three field quantities as a function of the coordinate Λ, this yields $\gamma = \tilde{\gamma}(\Lambda)$, $v = \tilde{v}(\Lambda)$ and $\theta = \tilde{\theta}(\Lambda)$.

Any self similar solution must satisfy the appropriate boundary conditions at the edges of the fan envelope, these conditions are

$$\tilde{\gamma}(\Lambda_1) = \gamma_T, \quad \tilde{v}(\Lambda_1) = v_T, \quad \tilde{\theta}(\Lambda_1) = \theta_T, \tag{6.27}$$

$$\tilde{\gamma}(\Lambda_2) = \gamma_2, \quad \tilde{v}(\Lambda_2) = 0, \quad \tilde{\theta}(\Lambda_2) = \hat{\theta}. \tag{6.28}$$

To determine the temperature $\tilde{\theta}(\Lambda)$ the unknown temperature function $\tilde{\theta}(\Lambda)$ is substituted into the positive characteristic direction associated with the Riemann invariant (3.65)

$$\Lambda = \frac{dx}{dt} = \sqrt{c_2^2 + \frac{c_2^4\alpha_2^2\tilde{\theta}(\Lambda)}{C_{\gamma 2}}}, \tag{6.29}$$

solving (6.29) for $\tilde{\theta}(\Lambda)$ yields

$$\tilde{\theta}(\Lambda) = \frac{C_{\gamma 2}}{c_2^4\alpha_2^2}\left(\Lambda^2 - c_2^2\right). \tag{6.30}$$

The two coordinates Λ_1 and Λ_2 can be expressed in terms of the temperatures θ_T and $\hat{\theta}$ via (6.27)$_3$ and (6.28)$_3$. From Figure 6.2 it is seen at $x = x_1^+$, for which $\Lambda = \Lambda_1$, that the temperature is $\theta = \theta_T$. Thus Λ_1 must satisfy

$$\Lambda_1 = \sqrt{\frac{c_2^4\alpha_2^2}{C_{\gamma 2}}\left(\frac{C_{\gamma 2}}{c_2^2\alpha_2^2} + \theta_T\right)}. \tag{6.31}$$

At the other edge of the fan $x = x_2^-$, $\Lambda = \Lambda_2$, and the temperature $\theta = \hat{\theta}$, thus

$$\Lambda_2 = \sqrt{\frac{c_2^4\alpha_2^2}{C_{\gamma 2}}\left(\frac{C_{\gamma 2}}{c_2^2\alpha_2^2} + \hat{\theta}\right)}. \tag{6.32}$$

This knowledge of the two slope coordinates Λ_1 and Λ_2 now allows for the determination of the other two unknown functions $\tilde{\gamma}(\Lambda)$ and $\tilde{v}(\Lambda)$.

To determine the strain $\gamma = \tilde{\gamma}(\Lambda)$ the Riemann invariant condition (3.62) is utilized, where within the fan envelope it requires

$$C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta_2^*}\right) + c_2^2\alpha_2\gamma_2 = C_{\gamma 2}\ln\left(\frac{\tilde{\theta}(\Lambda)}{\theta_2^*}\right) + c_2^2\alpha_2\tilde{\gamma}(\Lambda)\,. \tag{6.33}$$

Inserting the expression (6.30) into (6.33) allows for the strain $\tilde{\gamma}(\Lambda)$ to be expressed

$$\tilde{\gamma}(\Lambda) = \gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{c_2^4\alpha_2^2\hat{\theta}}{C_{\gamma 2}(\Lambda^2 - c_2^2)}\right). \tag{6.34}$$

The boundary conditions $(6.27)_1$ and $(6.28)_1$ require that $\tilde{\gamma}(\Lambda_1) = \gamma_T$ and $\tilde{\gamma}(\Lambda_2) = \gamma_2$. Inserting (6.31)-(6.32) into (6.34) one can demonstrate that both these conditions are satisfied.

Finally the velocity field $v = \tilde{v}(\Lambda)$ can be determined through the use of the Riemann invariant condition $(3.65)_2$

$$-\tilde{v}(\Lambda) - \sqrt{C_{\gamma 2}}\left[2\Phi(\tilde{\theta}(\Lambda)) + \Phi(0)\ln\left(\frac{\Phi(\tilde{\theta}(\Lambda)) - \Phi(0)}{\Phi(\tilde{\theta}(\Lambda)) + \Phi(0)}\right)\right] = \text{constant}. \tag{6.35}$$

Utilizing the initial conditions allows this condition to be written

$$\begin{aligned} -\tilde{v}(\Lambda) - \sqrt{C_{\gamma 2}}\left[2\Phi(\tilde{\theta}(\Lambda)) + \Phi(0)\ln\left(\frac{\Phi(\tilde{\theta}(\Lambda)) - \Phi(0)}{\Phi(\tilde{\theta}(\Lambda)) + \Phi(0)}\right)\right] &= \\ -\sqrt{C_{\gamma 2}}\left[2\Phi(\hat{\theta}) + \Phi(0)\ln\left(\frac{\Phi(\hat{\theta}) - \Phi(0)}{\Phi(\hat{\theta}) + \Phi(0)}\right)\right]&. \end{aligned} \tag{6.36}$$

From (6.36) the velocity $v = \tilde{v}(\Lambda)$ is

$$\tilde{v}(\Lambda) = 2\sqrt{C_{\gamma 2}}(\Phi(\hat{\theta}) - \Phi(\tilde{\theta}(\Lambda))) + \sqrt{C_{\gamma 2}}\Phi(0)\ln\left(\frac{\Phi(\hat{\theta}) - \Phi(0)}{\Phi(\hat{\theta}) + \Phi(0)}\right)$$
$$-\sqrt{C_{\gamma 2}}\Phi(0)\ln\left(\frac{\Phi(\tilde{\theta}(\Lambda)) - \Phi(0)}{\Phi(\tilde{\theta}(\Lambda)) + \Phi(0)}\right), \tag{6.37}$$

where

$$\Phi(\tilde{\theta}(\Lambda)) = \sqrt{\tilde{\theta}(\Lambda) + \frac{C_{\gamma 2}}{c_2^2\alpha_2^2}} = \sqrt{\frac{C_{\gamma 2}}{c_2^4\alpha_2^2}\Lambda^2}.$$

Inserting the expression $\Phi(\tilde{\theta}(\Lambda))$ into the equation the velocity is

$$\tilde{v}(\Lambda) = \frac{2C_{\gamma 2}}{c_2^2\alpha_2}(\Lambda_2 - \Lambda) + \frac{C_{\gamma 2}}{c_2\alpha_2}\left(\ln\left(\frac{\Lambda_2 - c_2}{\Lambda_2 + c_2}\right) - \ln\left(\frac{\Lambda - c_2}{\Lambda + c_2}\right)\right). \tag{6.38}$$

The boundary conditions $(6.27)_2$ and (6.28) require that $\tilde{v}(\Lambda_1) = v_T$ and $\tilde{v}(\Lambda_2) = 0$ inserting into (6.28) both these conditions are shown to be satisfied.

Thus, in summary, within the centered simple wave fan the strain, the velocity and temperature field are given by (6.34), (6.38), and (6.30) for all Λ obeying $\breve{c}_T \le \Lambda \le \breve{c}_{E_2}$.

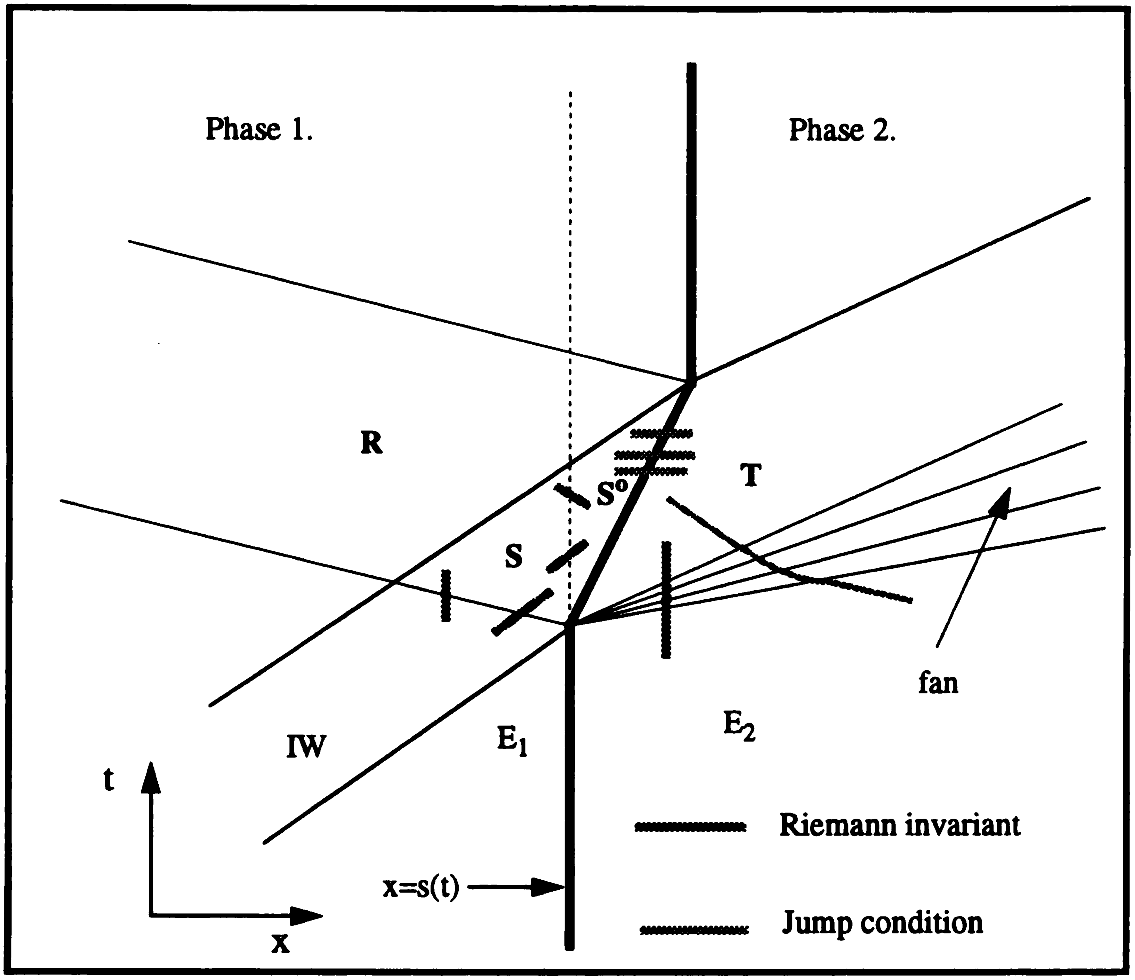

Figure 6.1 This is a graphical representation in the (xt)-plane of the initial interaction of a wave pulse with a stationary phase boundary in the fully thermodynamical theory. Regions E_1 and E_2 are the initial equilibrium states separated by the phase boundary at x=s(t). The incoming wave (IW) strikes the phase boundary setting it into motion, where $\dot{s} > 0$ is assumed. The IW-phase boundary interaction gives rise to the regions S, S^o and R in phase-1, and T and the simple centered wave (fan) in phase-2. The region R represents a reflected wave, while S arises from the interaction of the IW and the reflected wave. S^o is that material which has undergone a phase transformation from phase-1 to phase-2. The IW striking the phase boundary also produces a transmitted wave in phase-2, this is designated by the letter T. Finally the transition from the E_2 state to the T state is a simple centered wave, which requires $c_T < c_{E_2}$. The other possibility, that of a shock transition from the E_2 to the T-state, is not considered here but is discussed briefly in Appendix B. Comparing this diagram to figure 5.1 shows the additional complexity inherent in the fully thermodynamical theory.

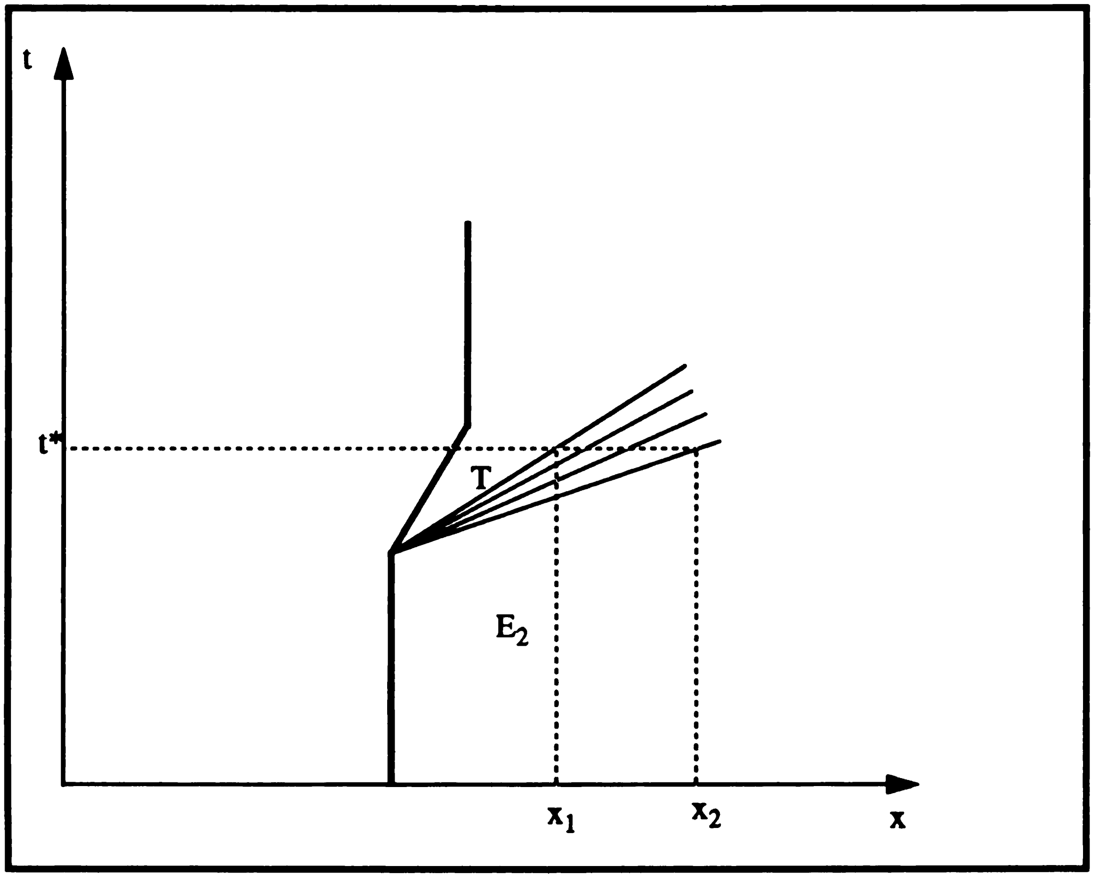

Figure 6.2 This is a representation of the fan transition in phase-2. The point (x_1,t^*) is located on the contiguous line between T and the fan, where $\frac{dx}{dt} = \Lambda_1 = \breve{c}_T$. The point (x_2,t^*) is on the line between the fan and the E_2 state, where $\frac{dx}{dt} = \Lambda_2 = \breve{c}_{E_2}$. Correct ordering of the speeds in the fan requires that $\breve{c}_{E_2} > \breve{c}_T$, which becomes an admissibility condition on the fan solution investigated in Section 7.3.

7. Construction of a Solution for Small Coefficient of Thermal Expansion

In this the chapter we examine the significance of the coefficient of thermal expansion for the initial interaction. Recall that the coefficient of thermal expansion, α_2, is a material constant responsible for the free energy being of the nonseparable form, and when α_2 vanishes the mechanical field variables γ, v decouple from the thermal field variable θ in the governing equations. In Chapter 4 the role of this material constant was analyzed for the initial equilibrium configurations, using the two part α_2 decomposition (3.92)-(3.94). This two part decomposition will continue to be utilized in what is to follow.

The purely mechanical problem was introduced in Chapter 5, and explicit results (5.3)-(5.6) were constructed for the initial interaction of a wave pulse with a phase boundary. In the fully thermomechanical problem posed in Chapter 6, fully explicit solutions are not obtained by virtue of the complexities of analyzing the master equation (6.14). For this problem we now wish to investigate the effects for small non- zero values of α_2, in order to garner insight into the first order temperature effects.

Recall that the two-phase model developed was for adiabatic motions, the possibility for heat transfer being excluded. Within this framework a finite value for the coefficient of thermal expansion results in the thermal and mechanical field quantities being coupled, and when this coefficient vanishes this coupling no longer exists. Ngan and Truskinovsky (1994) investigate problems for phase transforming solids in which the role of heat conduction (the Fourier model) is also accounted for. It is interesting to note in their development that the thermal conductivity is a coupling parameter similar to our α_2. Whereas here α_2 was the parameter enabling one to examine the link between adiabatic and purely mechanical motion, in their paper the thermal conductivity provides a heat conduction-adiabatic link.

Beginning with the equations which mathematically describe the initial interaction, (6.14)-(6.23), the leading order temperature effects are to be extracted via the assumption $\alpha_2 \ll 1$. Furthermore, it must be determined what factors, if any, ensure the retrieval of the previous results (5.3)-(5.6) when $\alpha_2 \to 0$. Accordingly, various perturbation and asymptotic procedures will be used to determine the leading order temperature effects[1].

Recall that once a solution for θ_T is found satisfying equation the master equation (6.14), then the other field quantities relating to the initial interaction may be determined explicitly from (6.16)-(6.23). Since it is not evident that a solution exists for the master equation, we propose to investigate solutions to (6.14) under the additional assumption that α_2 is small. In particular since $\alpha_2 = 0$ yields the separable theory for which $\theta_T = \hat{\theta}$, our interest is in solutions for which $\theta_T \to \hat{\theta}$ as $\alpha_2 \to 0$.

7.1 Perturbation Analysis of the Master Equation

The master equation (6.14) may be expressed in a more useful form, one in which all terms which have a temperature dependance are written on the left side of the equality sign

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[1] It should be pointed out since α_2 has units of reciprocal temperature, that these procedures formally require nondimensionalization of α_2 via multiplication by some characteristic temperature in the problem. It is in this sense that we operate, and which statements like α_2->0 need to be understood.

$$\sqrt{C_{\gamma 2}}\,(c_1 - \dot{s})\,(\vartheta\,(\theta_T) - \vartheta\,(\hat{\theta}))-\frac{C_{\gamma 2}(\dot{s}c_1 - c_2^2)}{c_2^2\alpha_2}\ln\left(\frac{\theta_T}{\hat{\theta}}\right) + c_2^2\alpha_2\left(\theta_T - \hat{\theta}\right) = \tag{7.1}$$

$$(\dot{s}c_1 - c_1^2)2\Delta\gamma + \dot{s}c_1\,(\gamma_1 - \gamma_2)\;.$$

The difficulty in finding a solution for this equation lies primarily in the non-linearity contained within the function $\vartheta\,(\theta)$, which from $(6.15)_1$is

$$\vartheta\,(\theta) \;=\; 2\Phi\,(\theta) + \Phi\,(0)\ln\left[\frac{\Phi\,(\theta) - \Phi\,(0)}{\Phi\,(\theta) + \Phi\,(0)}\right].$$

The function $\vartheta\,(\theta)$ contains $\Phi\,(\theta)$ in a linear and logarithmic manner, therefore the α_2 analysis will begin with $\Phi\,(\theta)$. Expanding the function $\Phi\,(\theta)$ about $\alpha_2 = 0$ produces

$$\Phi\,(\theta) \;=\; \frac{\sqrt{C_{\gamma 2}}}{c_2\alpha_2}\left(1 + \frac{\theta c_2^2\alpha_2^2}{C_{\gamma 2}}\right)^{\frac{1}{2}} \;=\; \frac{\sqrt{C_{\gamma 2}}}{c_2\alpha_2}\left[1 + \frac{\theta c_2^2\alpha_2^2}{2C_{\gamma 2}} - \frac{\theta^2 c_2^4\alpha_2^4}{8C_{\gamma 2}^2} + O(\alpha_2^6)\right]. \tag{7.2}$$

The logarithmic term of $\vartheta\,(\theta)$ contains $\Phi\,(\theta)$ both in the denominator and in the numerator. Use of (7.2) permits the expansion of the numerator and denominator about $\alpha_2 = 0$ which leads to

$$\Phi\,(\theta) - \Phi\,(0) \;=\; \frac{\sqrt{C_{\gamma 2}}}{c_2\alpha_2}\left[\frac{\theta c_2^2\alpha_2^2}{2C_{\gamma 2}} - \frac{\theta^2 c_2^4\alpha_2^4}{8C_{\gamma 2}^2} + O(\alpha_2^6)\right], \tag{7.3}$$

$$\Phi(\theta) + \Phi(0) = \frac{2\sqrt{C_{\gamma2}}}{c_2\alpha_2}\left[1 + \frac{\theta c_2^2\alpha_2^2}{4C_{\gamma2}} - \frac{\theta^2 c_2^4\alpha_2^4}{16C_{\gamma2}^2} + O(\alpha_2^6)\right], \tag{7.4}$$

upon which division of (7.3) by (7.4) produces

$$\frac{\Phi(\theta) - \Phi(0)}{\Phi(\theta) + \Phi(0)} = \frac{1}{2}\left[\frac{\theta c_2^2\alpha_2^2}{2C_{\gamma2}} - \frac{\theta^2 c_2^4\alpha_2^4}{8C_{\gamma2}^2} + O(\alpha_2^6)\right]\left[1 + \frac{\theta c_2^2\alpha_2^2}{4C_{\gamma2}} - \frac{\theta^2 c_2^4\alpha_2^4}{16C_{\gamma2}^2} + O(\alpha_2^6)\right]^{-1}. \tag{7.5}$$

Expanding the denominator of (7.5) and collecting terms of similar order in α_2 yields

$$\frac{\Phi(\theta) - \Phi(0)}{\Phi(\theta) + \Phi(0)} = \frac{\theta c_2^2\alpha_2^2}{4C_{\gamma2}} - \frac{\theta^2 c_2^4\alpha_2^4}{8C_{\gamma2}^2} + O(\alpha_2^6) = \frac{\theta c_2^2\alpha_2^2}{4C_{\gamma2}}\left[1 - \frac{\theta c_2^2\alpha_2^2}{2C_{\gamma2}} + O(\alpha_2^4)\right]. \tag{7.6}$$

Utilizing this result allows for the logarithmic part of the function $\vartheta(\theta)$ to be expressed

$$\begin{aligned} \ln\left(\frac{\Phi(\theta) - \Phi(0)}{\Phi(\theta) + \Phi(0)}\right) &= \ln\left(\frac{\theta c_2^2\alpha_2^2}{4C_{\gamma2}}\left[1 - \frac{\theta c_2^2\alpha_2^2}{2C_{\gamma2}} + O(\alpha_2^4)\right]\right) \\ &= \ln\left(\frac{\theta c_2^2\alpha_2^2}{4C_{\gamma2}}\right) + \ln\left(1 - \frac{\theta c_2^2\alpha_2^2}{2C_{\gamma2}} + O(\alpha_2^4)\right). \end{aligned} \tag{7.7}$$

The second logarithmic expression in (7.7) may be expanded about $\alpha_2 = 0$ using a Taylor series to the fourth order

$$\ln\left(1-\frac{\theta c_2^2\alpha_2^2}{2C_{\gamma 2}}+O(\alpha_2^4)\right) = -\frac{\theta c_2^2\alpha_2^2}{2C_{\gamma 2}}+O(\alpha_2^4). \qquad (7.8)$$

Consolidating results (7.2), (7.7) and (7.8) permits the function $\vartheta(\theta)$ to be written to the order $O(\alpha_2^3)$:

$$\vartheta(\theta) = \frac{2\sqrt{C_{\gamma 2}}}{c_2\alpha_2}+\frac{\sqrt{C_{\gamma 2}}}{c_2\alpha_2}\ln\left(\frac{\theta c_2^2\alpha_2^2}{4C_{\gamma 2}}\right)+\frac{\theta c_2\alpha_2}{2\sqrt{C_{\gamma 2}}}+O(\alpha_2^3). \qquad (7.9)$$

Equation (7.9) is the final form for $\vartheta(\theta)$ expansions, and will be used in what is to follow.

Note that $\vartheta(\theta)$ appears twice in equation (7.1), i.e. in the difference $\vartheta(\theta_T)-\vartheta(\hat{\theta})$. From the expansion (7.9), this difference in $\vartheta(\theta)$ results in the α_2^{-1} singularity canceling out

$$\vartheta(\theta_T)-\vartheta(\hat{\theta}) = \frac{\sqrt{C_{\gamma 2}}}{c_2\alpha_2}\ln\left(\frac{\theta_T}{\hat{\theta}}\right)+\frac{c_2\alpha_2}{2\sqrt{C_{\gamma 2}}}\left(\theta_T-\hat{\theta}\right)+O(\alpha_2^3). \qquad (7.10)$$

Use of (7.10) in (7.1) gives

$$\frac{C_{\gamma 2}(c_2(c_1-\acute{s})+c_2^2-\acute{s}c_1)}{c_2^2\alpha_2}\ln\left(\frac{\theta_T}{\hat{\theta}}\right)+\alpha_2\left(\frac{c_1-\acute{s}}{2c_2}+1\right)(\theta_T-\hat{\theta}) = \omega+O(\alpha_2^3), \qquad (7.11)$$

where $\omega\equiv(\acute{s}c_1-c_1^2)2\Delta\gamma+\acute{s}c_1(\gamma_1-\gamma_2)$, as defined previously in (6.27), depends upon the initial conditions, the material properties, and the phase boundary speed.To further simplify (7.11) let

$$\xi = \xi(\dot{s}, c_1, c_2) = (c_2(c_1 - \dot{s}) + c_2^2 - \dot{s}c_1) = (c_1 + c_2)(c_2 - \dot{s}), \tag{7.12}$$

which allows (7.11) to be expressed more simply

$$\frac{C_{\gamma 2}\xi}{c_2^2\alpha_2}\ln\left(\frac{\theta_T}{\hat{\theta}}\right) + \alpha_2\left(\frac{c_1 - \dot{s}}{2c_2} + 1\right)(\theta_T - \hat{\theta}) = \omega + O(\alpha_2^3). \tag{7.13}$$

Since a solution for θ_T to (7.13) is not obvious, we propose the following representation for θ_T:

$$\theta_T = \hat{\theta}[1 + \varphi]\exp\left(\frac{c_2^2\alpha_2\omega}{C_{\gamma 2}\xi}\right). \tag{7.14}$$

Thus φ by definition is $\varphi = \left(\theta_T/\hat{\theta}\right)\exp\left(-\frac{c_2^2\alpha_2\omega}{C_{\gamma 2}\xi}\right) - 1$. Hence if $\alpha_2 \to 0$ and $\theta_T \to \hat{\theta}$, then $\varphi \to 0$. Thus φ is expected to be a small quantity whose small α_2 representation remains to be determined. If both α_2 and φ vanish, then (7.14) demonstrates that the temperature $\theta_T \to \hat{\theta}$, the equilibrium temperature.

Inserting the proposed representation (7.14) into master equation (7.13) yields

$$\begin{aligned}\frac{\xi C_{\gamma 2}}{c_2^2 \alpha_2}\ln(1+\varphi) + \hat{\theta}\rho c_2^2 \alpha_2\left[\frac{c_1-\dot{s}}{2c_2}+1\right]\left(\exp\left(\frac{\rho c_2^2 \alpha_2 \omega}{C_{\gamma 2}\xi}\right)\right)\varphi = \\ \hat{\theta}\rho c_2^2 \alpha_2\left[\frac{c_1-\dot{s}}{2c_2}+1\right]\left(1-\exp\left(\frac{\rho c_2^2 \alpha_2 \omega}{C_{\gamma 2}\xi}\right)\right)+O(\alpha_2^3).\end{aligned} \tag{7.15}$$

Equation (7.15) is now regarded as an equation for the quantity φ. The leading order α_2 effect is determined by expanding (7.15) for small α_2, and since φ is expected to be small, the logarithm term is written using the expansion $\ln(1+\varphi) \approx \varphi + O(\varphi^2)$. From these operations one can determine φ from (7.15)

$$\varphi = \frac{-\omega c_2^5 \hat{\theta}\,(c_1 + 2c_2 - \dot{s})}{2\,(\xi C_{\gamma 2})^2}\alpha_2^3 + o(\alpha_2^3). \tag{7.16}$$

Here, as is standard, $o(z)$ denotes a quantity, that after division by z, vanishes as $z \to 0$. From (7.16) it is observed that the quantity φ is of the third order in α_2, thus, for $\alpha_2 \ll 1$, the logarithmic expansion for small φ is valid.

7.2 Small α_2 Decomposition of the Field Quantities

Inserting result (7.16) into (7.14) indicates that the temperature θ_T admits the expansion

$$\theta_T = \hat{\theta}\exp\left(\frac{c_2^2\alpha_2\omega}{C_{\gamma 2}\xi}\right)\left[1 - \frac{\omega c_2^5\hat{\theta}\,(c_1 + 2c_2 - \dot{s})}{2\,(\xi C_{\gamma 2})^2}\alpha_2^3 + o(\alpha_2^3)\right]. \tag{7.17}$$

From (7.17) it is observed that θ_T is dependent on the initial conditions by virtue of the quantity ω. The temperature θ_T may be thought of as a function of the forcing strain $\Delta\gamma$ and the phase boundary speed $\dot{s}$. From (7.17) we also see that the isothermal result, $\theta_T = \hat{\theta}$, is retrievable in the small α_2 limit; that is if $\alpha_2 \rightarrow 0$ then the temperature $\theta_T \rightarrow \hat{\theta}$. Invoking the decomposition (3.92)-(3.94) for the temperature θ_T, and expanding the expression $\exp\left(\frac{\omega c_2^2\alpha_2}{\xi C_{\gamma 2}}\right)$ about $\alpha_2 = 0$, the temperature θ_T can be expressed in the two part decomposition

$$\theta_T = \theta_T^o + \theta_T^{\alpha_2}, \tag{7.18}$$

where the two terms are found to be

$$\begin{aligned} \theta_T^o &= \hat{\theta}, \\ \theta_T^{\alpha_2} &= \frac{\omega c_2^2\hat{\theta}}{\xi C_{\gamma 2}}\alpha_2 + O(\alpha_2^2). \end{aligned} \tag{7.19}$$

Equation (7.18) represents a solution for the master equation (6.14) in the small α_2 limit. Recall that if a solution for θ_T has been determined then the remaining strains and velocities in the interaction region may be computed using (6.17)-(6.24). We now proceed with this process and determine the other eight field quantities.

Beginning with the equation for the strain γ_T, in the small α_2 limit γ_T can now be determined via (7.17). Inserting result (7.17) into equation (6.14), and once again invoking expansions for small α_2, the strain γ_T written in the two part decomposition is

$$\gamma_T = \gamma_T^o + \gamma_T^{\alpha_2}, \tag{7.20}$$

where the two components

$$\gamma_T^o = \gamma_2 - \frac{\omega}{\xi} = \gamma_2 + \frac{(c_1^2 - \dot{s}c_1)2\Delta\gamma - \dot{s}c_1(\gamma_1 - \gamma_2)}{(c_1 + c_2)(c_2 - \dot{s})}, \tag{7.21}$$

$$\gamma_T^{\alpha_2} = \frac{\omega c_2^3 \hat{\theta}(c_1 + 2c_2 - \dot{s})}{2\xi^2 C_{\gamma 2}} \alpha_2^2 + O(\alpha_2^3). \tag{7.22}$$

In (7.20)-(7.22) the strain γ_T has been decomposed into two distinct terms, (7.21) is that part of the strain γ_T that is entirely independent of α_2, while (7.22) is the part that is dependent on α_2. The strain component γ_T^o, representing the separable energy contribution to γ_T, is exactly the solution γ_T^{mech} (5.3) for the purely mechanical case outlined in Chapter 5. Thus, the separable energy contribution γ_T^o is equivalent to the purely mechanical contribution of the strain field γ_T. The expression $\gamma_T^{\alpha_2}$ represents the leading order temperature effect in the γ_T field, this thermal effect originates from the inclusion of the material constant α_2. It is observed from (7.22) that $\gamma_T^{\alpha_2}$ is quadratic in α_2, and thus $\gamma_T^{\alpha_2} \to 0$ as $\alpha_2 \to 0$. Thus, the purely mechanical field quantity is retrieved in the limit as the constant α_2 vanishes, i.e. $\alpha_2 \to 0 \Rightarrow \gamma_T \to \gamma_T^{o} = \gamma_T^{mech}$.

Proceeding with similar calculations for the other field variables using the temperature θ_T (7.19) in equations (6.18)-(6.24), along with the use of expansions for small α_2, one can write the other field quantities in the two part decomposition, as outlined in (3.92)-(3.94). These expressions for the field variables are given in the equations listed below, where all results are written in the form (8.18).

The velocity in the transmitted region, v_T:

$$v_T = v_T^{o} + v_T^{\alpha_2}, \tag{7.23}$$

where

$$v_T^{o} = c_1 c_2 \left[\frac{(\dot{s} - c_1)\, 2\Delta\gamma + \dot{s}\,(\gamma_1 - \gamma_2)}{(c_1 + c_2)\,(c_2 - \dot{s})} \right], \tag{7.24}$$

$$v_T^{\alpha_2} = -\frac{\omega c_2^3 \hat{\theta}(c_2^2 + c_1 \dot{s})}{2\xi^2 C_{\gamma 2}} \alpha_2^2 + O(\alpha_2^3). \tag{7.25}$$

The strain in region S°, γ_{S°:

$$\gamma_{S^\circ} = \gamma_{S^\circ}^{o} + \gamma_{S^\circ}^{\alpha_2}, \tag{7.26}$$

where

$$\gamma^{o}_{S^\circ} = \gamma_1 + \frac{2c_1c_2\Delta\gamma + \dot{s}\,[2c_1\Delta\gamma - c_2(\gamma_1 - \gamma_2)]}{(c_1 + c_2)\,(c_1 + \dot{s})}, \tag{7.27}$$

$$\gamma^{\alpha_2}_{S^\circ} = \frac{-\omega c_2^3\hat{\theta}}{2\xi^2 C_{\gamma 2}}\alpha_2^2 + O(\alpha_2^3). \tag{7.28}$$

The velocity in region S°, v_{S°:

$$v_{S^\circ} = v^{o}_{S^\circ} + v^{\alpha_2}_{S^\circ}, \tag{7.29}$$

where

$$v^{o}_{S^\circ} = \frac{\left[-2c_1^2\Delta\gamma + \dot{s}\,(-2c_2\Delta\gamma - c_2(\gamma_1 - \gamma_2))\right]c_1}{(c_1 + c_2)\,(c_1 + \dot{s})}, \tag{7.30}$$

$$v^{\alpha_2}_{S^\circ} = \frac{-\omega c_1 c_2^3\hat{\theta}}{2\xi^2 C_{\gamma 2}}\alpha_2^2 + O(\alpha_2^3). \tag{7.31}$$

Note that all of the above results (7.20)-(7.31) have a similar form, each quantity is decomposed into two decoupled terms, the first being entirely independent of the coupling constant α_2, representing the separable energy contribution, while the second term is that part of the field quantity that is the leading order α_2 effect. *In all these expressions the separable energy terms are exactly the same as those found in the purely mechanical problem* as outlined in Chapter 5, i.e.(5.3) -(5.6). Therefore, we see that $v^{o}_{T} = v^{mech}_{T}$,

$\gamma_{S^\circ}^{o} = \gamma_{S^\circ}^{mech}$, and $v_{S^\circ}^{o} = v_{S^\circ}^{mech}$, and thus *the separable theory predicts the same values for the field quantities* γ *and* v *as does the purely mechanical theory.* The second part of the decomposition, that which depends on α_2, represents the thermal effect on that field quantity, which may be further decomposed into the leading order temperature effect plus higher order terms. For the mechanical field variables, the strain and velocity terms, the leading order thermal effect is of the second order in α_2, while for the temperature θ_T the leading order thermal effect is linear in α_2.

We now examine the temperature for the material which has undergone a phase transformation, θ_{S°, and note that since this is not a mechanical field quantity, we have no previous information from the purely mechanical problem. Therefore, in its two part decomposition, the separable energy term has no mechanical analogue. From (6.24) the temperature θ_{S° can be written

$$\theta_{S^\circ} = T_1 + T_2 + (T_3 + T_4)\,T_5 \tag{7.32}$$

where we now rewrite the expressions for the T_i's in equation (7.32) by representing each field variable by its two part decomposition

$$T_1 = \frac{1}{C_{\gamma 1}}\left(\frac{c_2^2}{2}\left((\gamma_T^o - \gamma^* + \alpha_2\theta^*)^2 + 2(\gamma_T^o - \gamma^* + \alpha_2\theta^*)\gamma_T^{\alpha_2} + (\gamma_T^{\alpha_2})^2\right)\right.$$

$$\left. + C_{\gamma 1}(\theta_T^o + \theta_T^{\alpha_2}) + \frac{\hat{b}_2 - \hat{b}_1}{\rho}\right),$$

$$T_2 = \frac{-c_1^2}{2C_{\gamma 1}}\left[(\gamma_S^o)^2 + 2\gamma_S^o\gamma_S^{\alpha_2} + (\gamma_S^{\alpha_2})^2\right],$$

$$T_3 = \rho c_1^2(\gamma_S^o + \gamma_S^{\alpha_2}),$$

$$T_4 = \rho c_2^2\left[(\gamma_T^o - \gamma^* + \alpha_2\theta^*) + \gamma_T^{\alpha_2} - \alpha_2(\theta_T^o + \theta_T^{\alpha_2})\right],$$

$$T_5 = \frac{-1}{2\rho C_{\gamma 1}}\left[(\gamma_T^o - \gamma_S^o) + (\gamma_T^{\alpha_2} - \gamma_S^{\alpha_2})\right].$$

The explicit expression for the two part decomposition of θ_{S° is very large, and a more explict display of its form will not be displayed. Rather it is illuminating to consider the special case when the initial equilibrium configuration is mechanically neutral (viz. (4.19)). In this case, the two part decomposition for the temperature θ_{S°,

$$\theta_{S^\circ} = \theta_{S^\circ}^o + \theta_{S^\circ}^{\alpha_2} \tag{7.33}$$

gives

$$\theta_{S^\circ}^o = \hat{\theta} - \frac{1}{C_{\gamma 1}}\left(\frac{c_2^2}{2\dot{s}^2}(c_2^2 - \dot{s}^2)(\gamma_T^o - \gamma_2) - \frac{c_1^2}{2\dot{s}^2}(c_1^2 - \dot{s}^2)(\gamma_S^o - \gamma_1)\right) \qquad \text{(MN)}, \tag{7.34}$$

$$\theta_{S^\circ}^{\alpha_2} = \frac{c_2^2\alpha_2\hat{\theta}}{2\dot{s}^2 C_{\gamma 1}}\left(-c_2^2\frac{\omega}{\xi} + c_1^2(\gamma_S^o - \gamma_1)\right) + O(\alpha_2^2) \qquad \text{(MN)}. \tag{7.35}$$

Note from (7.34) that, in general, $\theta_{S^\circ}^o \neq \hat{\theta}$ indicating that changes in temperature can occur in the transformed material even in the $\alpha_2 \to 0$ limit. This issue of temperature changes for the purely separable energy problem will be addressed in more detail below.

Continuing with the mechanically neutral assumption a series of tedious algebraic manipulations on $\theta^o_{S^\circ}$, using the analogue of result (5.14), allows (7.34) to be written

$$\theta^o_{S^\circ} = \hat{\theta} + \frac{c_1^2 \Sigma(\Delta\gamma,\dot{s})}{C_{\gamma 1}(c_1+c_2)(c_1+\dot{s})(c_2-\dot{s})} \qquad (\mathrm{MN}), \qquad (7.36)$$

where the function $\Sigma(\Delta\gamma,\dot{s})$ was defined earlier in the document as equation (5.15)

$$\begin{aligned}\Sigma(\Delta\gamma,\dot{s}) = {} & \dot{s}^2[2\Delta\gamma((c_1-c_2)\Delta\gamma - c_2(\gamma_1-\gamma_2))] + \\ & -\dot{s}\left[2(c_1-c_2)^2\Delta\gamma^2 - 2c_2(c_1-c_2)(\gamma_1-\gamma_2)\Delta\gamma + c_2^2(\gamma_1-\gamma_2)^2\right] \\ & -[2c_1c_2\Delta\gamma((c_1-c_2)\Delta\gamma - c_2(\gamma_1-\gamma_2))] .\end{aligned}$$

Note that, as required, the temperature θ^o_S is independent of the energy coupling constant α_2. Comparing a separable material with the purely mechanical material result (7.36) presents one of the fundamental differences between the two cases, the separable material accounts for changes in temperature arising from a phase transformation. The function $\Sigma(\Delta\gamma,\dot{s})$ was introduced in Chapter 5 and analyzed by Pence (1991b), thus one may garner information on the transformed material's temperature changes via (7.36) in conjunction with the $\Sigma(\Delta\gamma,\dot{s})$ analysis.

The representation for $\theta^o_{S^\circ}$ in (7.34) is somewhat paradoxical in that it contains the function $\Sigma(\Delta\gamma,\dot{s})$ which arose previously in (5.14) for the purely mechanical theory. Furthermore, under the assumption that the initial conditions are Maxwellian, result (5.16) provided a relationship between the function $\Sigma(\Delta\gamma,\dot{s})$ and the purely mechanical dissipation function. Thus from (5.16) and (7.13) one may conclude that if the initial conditions are *both* mechanically neutral and Maxwellian then one may utilize the dissipation function from the purely mechanical theory to express the temperature $\theta^o_{S^\circ}$ as

$$\theta^o_{S^\circ} = \hat{\theta} + \frac{1}{\rho C_{\gamma 1}\dot{s}} D(\Delta\gamma,\dot{s}) \qquad (\mathrm{OB}), \tag{7.37}$$

where we have used notation to remind us that simultaneous satisfaction of MN and MX equilibrium conditions are associated with the extremely special OB states. Alternatively this result can be rewritten as

$$D(\Delta\gamma,\dot{s}) = \rho C_{\gamma 1}\dot{s}(\theta^o_{S^\circ} - \hat{\theta}) \qquad (\mathrm{OB}). \tag{7.38}$$

Since the dissipation function $D(\Delta\gamma,\dot{s})$ is independent of α_2, result (7.38) demonstrates one of the novel abilities of the free energy model used in this document, namely in the case of a separable material, $\alpha_2 = 0$, (7.38) accounts for the expected changes in temperature for motions which are dissipative.

Previously it has been shown that if the material is separable then the mechanical motions decouple from thermal effects, yielding a purely mechanical problem and the associated thermal problem. Result (7.38) demonstrates one way in which the mechanical fields influence the thermal fields for a separable material, for once the mechanical field variables for the problem have been determined, and thus the dissipation function

$D(\Delta\gamma,\dot{s})$ is known, one may then proceed to calculate the thermal field variables. Furthermore if, as in a purely mechanical setting, one assumes a positive dissipation criteria, then (7.38) shows that the temperature of the material undergoing a phase transformation may only increase.

Thus, for $\alpha_2 = 0$ we do have a theory which is purely mechanical, in the sense that information about the temperature fields are not needed to determine the mechanical fields. Under such a separable energy criteria one may, at first glance, improperly interpret the problem as being isothermal, which from the result (7.38), is clearly not always the case. As seen from (7.38) isothermal motions occur only for nondissipative motions, i.e. those motions for which $D(\Delta\gamma,\dot{s}) = 0$, and thus are a subset of the solution set for the separable energy theory.

7.3 Existence of Fan

With the solution in hand we now wish to determine any necessary criteria for the existence of a fan transition in phase-2. Recall from (6.31) and (6.32) that a necessary and sufficient condition for the construction of this fan solution is that $\theta_T \le \hat{\theta}$. It follows from (7.18) and (7.19) that $\theta_T = \theta_T^o + \theta_T^{\alpha_2}$ where $\theta_T^o = \hat{\theta}$ so that the associated existence condition reduces to $\theta_T^{\alpha_2} < 0$.

In the absence of a simple explicit form for $\theta_T^{\alpha_2}$, we restrict attention to the small α_2 limit. In this limit, which makes contact with the separable energy theory corresponding to purely mechanical determination of strain and velocity, it follows from (6.3) that the phase boundary speed $\dot{s}$ must obey $\dot{s} < c_2$. In the small α_2 limit, the leading order α_2

effect for $\theta_T^{\alpha_2}$ is given in $(7.19)_2$, so that the requirement that $\theta_T^{\alpha_2} < 0$ for small α_2 is

$$\frac{\omega c_2^2 \hat{\theta}}{\xi C_{\gamma 2}} \alpha_2 < 0. \tag{7.39}$$

Since $\hat{\theta} > 0$, $C_{\gamma 2} > 0$ and α_2 tends to zero through positive values, one may draw that (7.39) is equivalent to the requirement that $\frac{\omega}{\xi} \leq 0$, where we recall that ω and ξ are given by (7.23) and (7.12). The latter, $\xi = \xi(\dot{s}, c_1, c_2) = (c_1 + c_2)(c_2 - \dot{s})$, shows that $\xi \geq 0$ since $\dot{s} < c_2$ in the $\alpha_2 \rightarrow 0$ limit for fan existence. Therefore from (7.39) the criterion for the existence of a fan is

$\omega < 0$ or

$$(\dot{s}c_1 - c_1^2) 2\Delta\gamma + \dot{s}c_1 (\gamma_1 - \gamma_2) < 0. \tag{7.40}$$

This condition may be interpreted in various ways, in particular it may be used to obtain a restriction on $\dot{s}$, namely

$$\begin{aligned} \dot{s} &< \frac{-2\Delta\gamma c_1}{(\gamma_2 - \gamma_1) - 2\Delta\gamma} \quad \text{if} \quad \gamma_2 - \gamma_1 - 2\Delta\gamma < 0, \\ \dot{s} &> \frac{-2\Delta\gamma c_1}{(\gamma_2 - \gamma_1) - 2\Delta\gamma} \quad \text{if} \quad \gamma_2 - \gamma_1 - 2\Delta\gamma > 0. \end{aligned} \tag{7.41}$$

Now $\gamma_2 > \gamma_1$ and since the driving strain increment $\Delta\gamma$ would normally be much less than $\gamma_2 - \gamma_1$, the standard case in (7.41) would in general be $(7.41)_2$. Since it is already required that $0 < \dot{s} < c_2$ it follows that $(7.41)_2$ may or may not further restrict the phase boundary velocity. In particular if $\Delta\gamma > 0$ then $(7.41)_2$ provides no additional restrictions. However if $\Delta\gamma < 0$ then $(7.41)_2$ restricts the lowest phase boundary speed to a finite positive value.

Figure 7.1 is a schematic diagram in the $(\Delta\gamma, \dot{s})$ -plane for the region satisfying the fan criterion (7.41), this figure only considers positive values of $\dot{s}$. This region lies above the curve $\omega = 0$, where the equation for the curve is given by (6.26). Also shown in Figure 7.1 is the admissibility region for the purely mechanical problem defined by (5.17), this region was previously displayed in Figure 5.2. In Figure 7.1 this admissability region is below the curve $\Sigma = 0$ and above the line $\dot{s} = 0$, and from Figure 7.1 we see that the curve $\omega = 0$ is contained within the admissibility region. Therefore the area between the two curves $\Sigma = 0$ and $\omega = 0$ defines the region for which the construction of a centered simple wave fan solution is admissible for the $\alpha_2 \rightarrow 0$ limit.

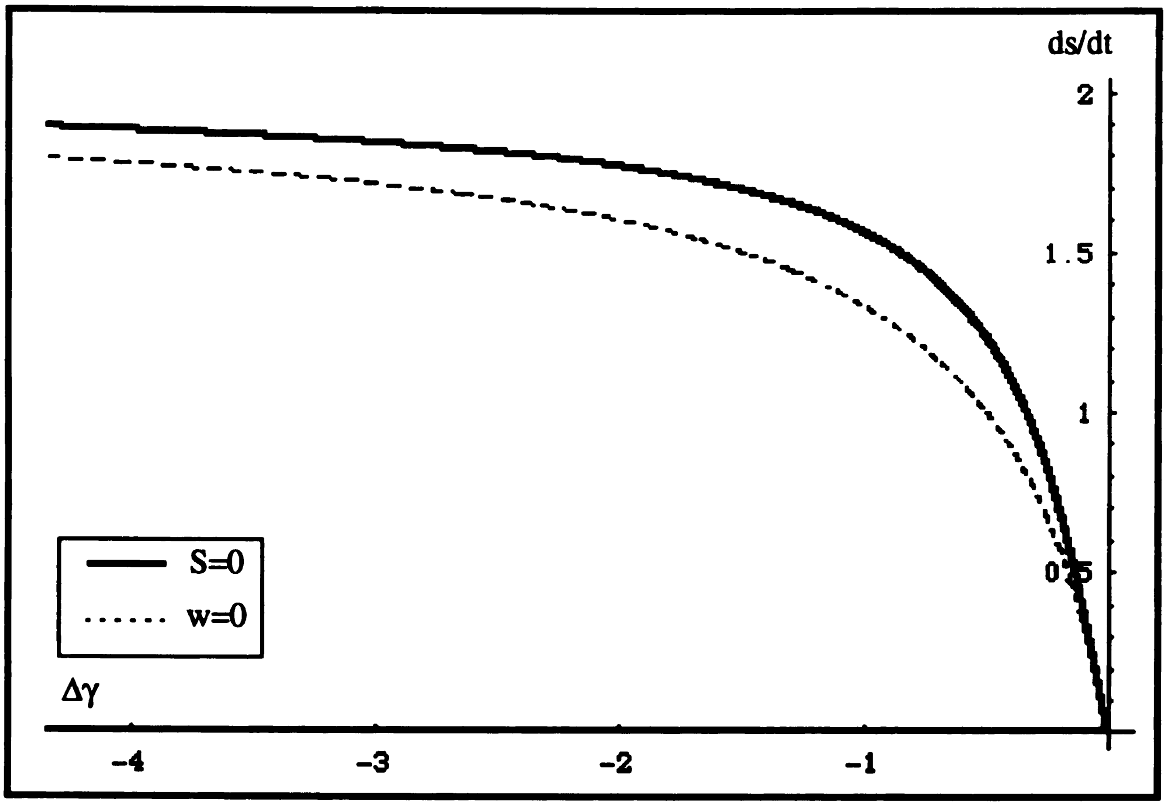

Figure 7.1 This is a schematic plot which shows the admissible region for a centered simple wave for the case where $c_1 = c_2$. The region that lies between the line $\dot{s} = 0$ and the curve $\Sigma = 0$ is the admissible region for the purely mechanical case with Maxwellian initial conditions as previously encountered in Figure 5.2. The region above the curve $\omega = 0$ is the region in which the centered simple wave may exist. Therefore the region of existence for the centered simple wave is the area between the two curves. Values for the material parameters were chosen to be $c = 2$ and $\gamma_2 - \gamma_1 = 5$.

8. Entropy Production and Dissipation

In Chapter 7 it was shown that if the phase boundary speed is treated as a free parameter then it parameterizes a family of solutions involving a centered simple wave fan. It was the case that an explict solution, albeit a family of solutions, was determined only when considering the small α_2 limit, which in turn provided insight into the leading order thermal effects. Recall that the second law of thermodynamics $(2.6)_4$ was not utilized in determining the family of solutions, although it is one of the four governing field requirements in each phase of the material.Thus, it is natural to inquire as to what restrictions this inequality places on the set of possible solution candidates in $(\Delta\gamma, \dot{s})$ -space.

It is acknowledged that such a requirement is not directly given in the purely mechanical theory, but is provided indirectly through the positive dissipation criteria requirement, more specifically the dissipation function (5.9) must be nonnegative $D(\Delta\gamma, \dot{s}) \geq 0$. In this chapter we investigate any relationships that may exist between the positive dissipation requirement for a purely mechanical material and the restrictions imposed by the second law of thermodynamics for the fully thermal materials, with emphasis on the separable material limit.

8.1 The Second Law of Thermodynamics.

The second law of thermodynamics in the absence of heat flux and internal energy sources states that the rate of change in entropy for a system must be nonnegative during all processes, globally this requires

$$\frac{d}{dt}\int_V \eta dV \geq 0. \tag{8.1}$$

The domain under consideration is a bar which contains a propagating surface of discontinuity, the appropriate form for the above equation is written

$$\int_0^{s(t)} \frac{d\eta}{dt}dx + \int_{s(t)}^{h} \frac{d\eta}{dt}dx - \dot{s}[[\eta]] \geq 0. \tag{8.2}$$

From (8.2) it is observed that the time rate of change in entropy arises from two distinct sources, those resulting from local thermomechanical processes in the bulk material, and that contribution from the movement of the surface of discontinuity through the domain. Considering (8.2) in its local form one retrieves $(2.6)_4$ and $(2.7)_4$. Note that the jump in entropy across a surface of discontinuity is not required to vanish, and thus this jump condition must be applied across all phase boundaries, and if present, any shocks within the domain. However, by use of the Riemann invariants (3.62), the jump in entropy vanishes across all contact discontinuities.

Consider the initial interaction of the wave pulse with the stationary phase boundary, and focus on the period of time for which the phase boundary is still in motion. To implement equation (8.2) during this interval requires the consideration of 7 separate regions within the bar: the parent phase equilibrium state, the region containing the incoming wave, the regions labelled S, T and S^o(the material having undergone a phase transformation), the phase-2 equilibrium state, and the region containing the centered simple wave fan. Figure 6.1 depicts the initial interaction and shows the seven regions. Invoking restriction (8.2) to the various regions and the surfaces separating adjacent regions, one recognizes that all the integral terms on either side of the phase boundary vanish as do the terms involving jumps across all contact discontinuities. Therefore the only nonvanishing contribution to (8.2) is that associated with the jump in entropy across the phase boundary, thus (8.2) reduces to

$$-\dot{s}\,[\eta\,(\gamma_T, \theta_T) - \eta\,(\gamma_{S^\circ}, \theta_{S^\circ})] \geq 0, \tag{8.3}$$

where the entropy function (3.19) is used to express

$$\begin{aligned} \eta\,(\gamma_{S^\circ}, \theta_{S^\circ}) &= \rho C_{\gamma 1} \ln\left(\frac{\theta_{S^\circ}}{\theta^*}\right) + \tilde{k}_1, \\ \eta\,(\gamma_T, \theta_T) &= \rho C_{\gamma 2} \ln\left(\frac{\theta_T}{\theta^*}\right) + \rho c_2^2 \alpha_2 (\gamma_T - \gamma^*) + \frac{\rho \lambda_T}{\theta^*} + \tilde{k}_1. \end{aligned} \tag{8.4}$$

Inequality (8.3) implies that $\eta_{S^\circ} \geq \eta_T$ since $\dot{s} > 0$, indicating as the material transforms, from phase-2 in the T-region to phase-1 in the S^o-region, that the transforming material's field variables must change in a manner such that the difference in entropy is nonnegative, i.e.

$$\eta\,(\gamma_{S^\circ}, \theta_{S^\circ}) - \eta\,(\gamma_T, \theta_T) \geq 0. \tag{8.5}$$

Through the use of the Riemann invariant (3.62) between regions T and the material in the phase-2 equilibrium configuration one may show that $\eta\,(\gamma_T, \theta_T) = \eta\,(\gamma_2, \theta_2)$, which written out in its full form is

$$\begin{aligned}&\rho C_{\gamma 2}\ln\left(\frac{\theta_T}{\theta^*}\right)+\rho c_2^2\alpha_2(\gamma_T-\gamma^*)+\frac{\rho\lambda_T}{\theta^*}+\tilde{k}_1=\\&\rho C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right)+\rho c_2^2\alpha_2(\gamma_2-\gamma^*)+\frac{\rho\lambda_T}{\theta^*}+\tilde{k}_1.\end{aligned}\tag{8.6}$$

Equation (8.6) provides a relationship between the entropy in region T and the initial configuration within the bar, while (8.5) restricts the difference in entropy between T and S^0. Therefore, instead of using the entropy η_T in inequality (8.5) we choose to use that from the phase-2 equilibrium configuration, via equality (8.6), and thus write restriction (8.5) as an equation between the regions S^0 and the phase-2 equilibrium state. Therefore, condition (8.5) is equivalent to

$$C_{\gamma 1}\ln\left(\frac{\theta_{S^\circ}}{\theta^*}\right)-C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right)-c_2^2\alpha_2(\gamma_2-\gamma^*)-\frac{\lambda_T}{\theta^*}\geq 0.\tag{8.7}$$

The inequality (8.7) is a restriction on the temperature θ_{S°, all other field quantities being prescribed by specification of the initial conditions and material parameters. This restriction (8.7) is equivalently expressed

$$\theta_{S^\circ}\geq\hat{\theta}^{\frac{C_{\gamma 2}}{C_{\gamma 1}}}\theta^{*\,1-\frac{C_{\gamma 2}}{C_{\gamma 1}}}\exp\left\{\frac{c_2^2\alpha_2(\gamma_2-\gamma^*)}{C_{\gamma 1}}+\frac{\lambda_T}{C_{\gamma 1}\theta^*}\right\}.\tag{8.8}$$

Thus, given an admissible initial data set $(\gamma_1, \gamma_2, \hat{\theta})$, the second law of thermodynamics states that all allowable motions must adhere to condition (8.8), where (8.8) restricts the possible range of values of the temperature θ_{S°. It is interesting to note that since θ_{S° is the temperature of the material which has undergone a phase transformation, (8.8) is a restriction on the transformed material's temperature. It is also interesting to consider that the second law of thermodynamics, a dynamic balance requirement without analogue in the purely mechanical setting, places restrictions on a thermal field variable, a field variable not having any mechanical analogue.

We now focus our attention on the special case when the different phases have identical specific heats, $C_{\gamma 1} = C_{\gamma 2}$, then (8.8) simplifies to

$$\theta_{S^\circ} \geq \hat{\theta} \exp\left\{ \frac{c_2^2 \alpha_2}{C_\gamma}(\gamma_2 - \gamma^*) + \frac{\lambda_T}{C_\gamma \theta^*} \right\} \equiv \theta_{S^\circ}\Big|_{\text{lower bound}} \qquad (C_{\gamma 1} = C_{\gamma 2}) . \qquad (8.9)$$

Table 5 summarizes the relation between the lower bound value of θ_{S° and the initial temperature $\hat{\theta}$ as a function of initial strain γ_2.

Table 5: Lower bound temperature of transformed material $\theta_{S^\circ}\big|_{\text{lower bound}}$ when $C_{\gamma 1} = C_{\gamma 2} = C_\gamma$.

Value of γ_2	Temperature $\theta_{S^\circ}\big|_{\text{lower bound}}$
$\gamma_2 < \gamma^* - \frac{\lambda_T}{c_2^2\alpha_2\theta^*}$	$\theta_{S^\circ}\big|_{\text{lower bound}} < \hat{\theta}$
$\gamma_2 = \gamma^* - \frac{\lambda_T}{c_2^2\alpha_2\theta^*}$	$\theta_{S^\circ}\big|_{\text{lower bound}} = \hat{\theta}$
$\gamma_2 > \gamma^* - \frac{\lambda_T}{c_2^2\alpha_2\theta^*}$	$\theta_{S^\circ}\big|_{\text{lower bound}} > \hat{\theta}$

As shown in Chapter 6, to explicitly calculate the temperature θ_{S° one uses (6.20) after determining a solution for the master equation (6.14) for the temperature θ_T. In order to further quantify the restriction (8.7) we now consider the special case where the coefficient $\alpha_2 \ll 1$. Inserting the decomposition $\theta_{S^\circ} = \theta^o_{S^\circ} + \theta^{\alpha_2}_{S^\circ}$ into (8.7) yields

$$C_{\gamma 1}\ln\left(\frac{\theta^o_{S^\circ}}{\theta^*}\right) + C_{\gamma 1}\ln\left(1 + \frac{\theta^{\alpha_2}_{S^\circ}}{\theta^o_{S^\circ}}\right) - C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) - c_2^2\alpha_2(\gamma_2 - \gamma^*) - \frac{\lambda_T}{\theta^*} \geq 0. \qquad (8.10)$$

All further discussion of (8.10) appears in the following sections for the case $\alpha_2 \to 0$ and $\alpha_2 \ll 1$.

8.2 The Entropy Restriction for Separable Materials

Recall that the limit $\alpha_2 \to 0$ reduces the free energy to its separable form, in which case (8.10) reduces to

$$C_{\gamma 1}\ln\left(\frac{\theta^{o}_{S^{o}}}{\theta^{*}}\right) - C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta^{*}}\right) - \frac{\lambda_T}{\theta^{*}} \geq 0. \tag{8.11}$$

Once again considering the special case where the two phases have the same specific heats then inequality (8.11) simplifies into the form

$$\theta^{o}_{S^{o}} \geq \hat{\theta}\exp\left\{\frac{\lambda_T}{C_\gamma \theta^{*}}\right\} \equiv \theta^{o}_{S^{o}}\Big|_{\text{lower bound}} \qquad (C_{\gamma 2} = C_{\gamma 1})\,. \tag{8.12}$$

The inequality (8.12) demonstrates that if the latent heat vanishes $(\lambda_T = 0)$ then the transformed material's temperature can not decrease below the initial equilibrium temperature $\hat{\theta}$. For the case of a separable material, the value of the quantity $\frac{\lambda_T}{C_\gamma \theta^{*}}$ determines the magnitude of the temperature $\theta^{o}_{S^{o}}\Big|_{\text{lower bound}}$. As was the case for $\alpha_2 \to 0$ a table is constructed which outlines the range of values for (8.12) which the temperature $\theta^{o}_{S^{o}}\Big|_{\text{lower bound}}$ may achieve, these values being listed in Table 6.

Table 6: Lower bound temperature $\theta^{o}_{S^{\circ}}\big|_{\text{lower bound}}$ for separable material when $C_{\gamma 1} = C_{\gamma 2} = C_{\gamma}$

Magnitude of $\lambda_T / C_\gamma \theta^*$	Temperature $\theta^{o}_{S^{\circ}}\big|_{\text{lower bound}}$
$\dfrac{\lambda_T}{C_\gamma \theta^*} < 0$	$\theta^{o}_{S^{\circ}}\big|_{\text{lower bound}} < \hat{\theta}$
$\dfrac{\lambda_T}{C_\gamma \theta^*} > 0$	$\theta^{o}_{S^{\circ}}\big|_{\text{lower bound}} > \hat{\theta}$

Recall from (3.80) that if $\lambda_T > 0$ then the $2 \rightarrow 1$ transformation is exothermic, whereas if $\lambda_T < 0$ then the transformation is endothermic. If we consider $C_\gamma \theta^* > 0$, then from Table 6 an exothermic transformation coincides with the transformed region's lower bound temperature being greater than its initial equilibrium temperature, which represents a heating of the transformed material. Similarly an endothermic reaction corresponds to transformed region's lower bound temperature being less than its initial equilibrium temperature, a cooling of the transformed material.

Consider the results found for the special case of mechanically neutral initial conditions (4.19)-(4.25), this allows $\theta^{o}_{S^{\circ}}$ to be expressed in terms of the function $\Sigma\,(\Delta\gamma,\,\dot{s})$ by means of (7.36):

$$\theta^{o}_{S^{\circ}} = \hat{\theta} + \frac{c_1^2 \Sigma\,(\Delta\gamma,\dot{s})}{C_{\gamma 1}\,(c_1 + c_2)\,(c_1 + \dot{s})\,(c_2 - \dot{s})} \qquad (\mathrm{MN})\,.$$

Substituting this expression into (8.11) yields

$$\ln\left(\frac{\hat{\theta}}{\theta^*}+\frac{c_1^2\Sigma(\Delta\gamma,\dot{s})}{\theta^* C_{\gamma 1}(c_1+c_2)(c_1+\dot{s})(c_2-\dot{s})}\right)-\frac{C_{\gamma 2}}{C_{\gamma 1}}\ln\left(\frac{\hat{\theta}}{\theta^*}\right)-\frac{\lambda_T}{C_{\gamma 1}\theta^*}\geq 0 \qquad \text{(MN)},$$

which in turn reduces to

$$\frac{c_1^2\Sigma(\Delta\gamma,\dot{s})}{C_{\gamma 1}(c_1+c_2)(c_1+\dot{s})(c_2-\dot{s})}\geq$$
$$\theta^*\left(\exp\left\{\frac{C_{\gamma 2}}{C_{\gamma 1}}\ln\left(\frac{\hat{\theta}}{\theta^*}\right)+\frac{\lambda_T}{C_{\gamma 1}\theta^*}\right\}-\frac{\hat{\theta}}{\theta^*}\right) \qquad \text{(MN)}. \tag{8.13}$$

The inequality (8.13), along with the condition $\dot{s}>0$, restricts the set of solutions in $(\Delta\gamma, \dot{s})$ -space. Recall from Chapter 5, in a purely mechanical setting, a similar restriction was derived, e.g. $\dot{s}\Sigma(\Delta\gamma, \dot{s})\geq 0$. This was a consequence of the assumption that all motions must have nonnegative dissipation, and like (8.13), reduced the set of solutions in the $(\Delta\gamma, \dot{s})$ -space.

If we now consider the inequality (8.13) for the particular case $C_{\gamma 2} = C_{\gamma 1}$ and $\lambda_T = 0$, then since $\dot{s}\leq c_2$ we find that

$$\Sigma(\Delta\gamma,\dot{s})\geq 0 \qquad (C_{\gamma 2}=C_{\gamma 1}, \lambda_T=0), \tag{8.14}$$

which is essentially the same restriction found for the purely mechanical problem (see (5.17)). However it is noted that one cannot directly compare the two conditions, because result (5.17) was derived for the Maxwellian initial state while (8.14) is for the mechanically neutral initial state.

A more fundamental and less restricted result occurs for the case in which the initial state is omnibalanced. In Chapter 7 it was shown for an omnibalanced initial configuration that $\theta^{o}_{s_o}$ can be written in terms of the purely mechanical dissipation function $D(\Delta\gamma,\dot{s})$ via (7.37). This reduces (8.11) to

$$\frac{D(\Delta\gamma,\dot{s})}{\dot{s}} \geq \rho C_{\gamma 1}\theta^{*}\left\{\exp\left\{\frac{C_{\gamma 2}}{C_{\gamma 1}}\ln\left(\frac{\hat{\theta}^{OB}}{\theta^{*}}\right)+\frac{\lambda_T}{C_{\gamma 1}\theta^{*}}\right\}-\frac{\hat{\theta}^{OB}}{\theta^{*}}\right\} \qquad (OB)\,. \qquad (8.15)$$

Recall however that an OB-initial state must involve initial temperatures as given by $(4.32)_1$. Substitution from $(4.32)_1$ and invoking $\rho C_{\gamma 1}\dot{s} > 0$ in (8.15) gives

$$D(\Delta\gamma,\dot{s}) \geq 0 \qquad (OB)\,. \qquad (8.16)$$

Thus the positive dissipation criterion in the purely mechanical description has a strict thermodynamic basis in terms of $(2.7)_4$ in the separable material limit. In view of the complexity encountered thus far in interpreting second law issues, any further consideration into these issues would most profitably restrict attention to omnibalanced states. In particular, the first order α_2-correction to (8.16) for the omnibalanced state is addressed in the next section.

8.3 The Entropy Restriction for Fully Thermal Materials

Our previous discussion has established that the $\alpha_2 \to 0$ admissibility region coincides with the admissibility region for the purely mechanical problem provided that the thermomechanical problem had omnibalanced conditions. It is of interest to determine how the admissability region changes with the consideration of thermal effects. In what follows we address this issue and concentrate on OB initial states when $c_1 = c_2$.

To determine how the $\alpha_2 \to 0$ admissibility region changes for small but finite α_2, we evaluate (8.10) along all of the boundaries of the $\alpha_2 = 0$ admissibility region. Recall that these boundaries are defined by (5.17), which gives the line $\dot{s} = 0$ and the curve $\Sigma = 0$. We here evaluate (8.10) along $\Sigma = 0$. By definition (5.17) the quantity

$$C_{\gamma 1}\ln\left(\frac{\theta^{o}_{S^\circ}}{\theta^*}\right) - C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) - \frac{\lambda_T}{\theta^*}$$

vanishes along $\Sigma = 0$. Therefore to determine the thermal correction to the admissible region we need only evaluate the remaining expression in (8.10) along $\Sigma = 0$. Define the function z as

$$z \equiv C_{\gamma 1}\ln\left(1 + \frac{\theta^{\alpha_2}_{S^\circ}}{\theta^{o}_{S^\circ}}\right) - c_2^2\alpha_2(\gamma_2 - \gamma^*), \tag{8.17}$$

whereby evaluating z along $\Sigma = 0$ provides the thermal correction. Locations where $z > 0$ are points on the boundary where the purely mechanical admissibility criterion and the thermal admissibility criterion are satisfied. Similarly at those points where $z < 0$ the purely mechanical admissibility criterion is satisfied, but the thermal admissibility criterion is not satisfied. In this manner one can show where addition of the thermal correction (8.17) causes the admissibility region to “grow” $(z > 0)$ and “shrink” $(z > 0)$ in a point wise fashion.

From (7.35) the temperature $\theta_{S^\circ}^{\alpha_2}$ can be expanded to the first order in α_2, which in turn allows for the logarithmic expression in (8.17) to be expanded

$$C_{\gamma 1}\ln\left(1+\frac{\theta_{S^\circ}^{\alpha_2}}{\theta_{S^\circ}^{o}}\right) = C_{\gamma 1}\frac{\theta_{S^\circ}^{\alpha_2}}{\hat{\theta}} + O(\alpha_2^2), \tag{8.18}$$

where we evaluated (7.37) along $\Sigma = 0$ to write $\theta_{S^\circ}^{o} = \hat{\theta}$. Using (7.35) and (8.18) in (8.17) the function z can be expressed

$$z = \frac{c^2\alpha_2}{2\dot{s}^2}\left(c^2 2\Delta\gamma + \frac{c^3\dot{s}(\gamma_2-\gamma_1)}{(c^2-\dot{s}^2)} - 2\dot{s}^2(\gamma_2-\gamma^*)\right) + O(\alpha_2^2),$$

where we have used (7.27) and the definitions for ω and ξ which are found in Chapter 7. Focusing on the leading order α_2 effect, we note the coefficient $\dfrac{c^2\alpha_2}{2\dot{s}^2}$ is positive when considering $0 < \alpha_2 \ll 1$, hence to determine the sign of z we need only consider the expression

$$c^2 2\Delta\gamma + \frac{c^3\dot{s}(\gamma_2-\gamma_1)}{(c^2-\dot{s}^2)} - 2\dot{s}^2(\gamma_2-\gamma^*) \tag{8.19}$$

evaluated along the curve $\Sigma = 0$. Using (5.18) the curve $\Sigma = 0$ yields the expression for

the strain increment $\Delta\gamma$

$$2\Delta\gamma = \frac{-\acute{s}c\,(\gamma_2-\gamma_1)}{(c^2-\acute{s}^2)},$$

which when inserted into (8.19) yields

$$\operatorname{sign}[z|_{\Sigma=0}] = \operatorname{sign}\left[-2\acute{s}^2(\gamma_2-\gamma^*)\right]. \tag{8.20}$$

Using the OB phase-2 strain $(4.31)_2$ in (8.20) yields

$$\operatorname{sign}[z|_{\Sigma=0}] = \operatorname{sign}\left[\frac{2\acute{s}^2\lambda_T}{\alpha_2 c^2\theta^*}\right]. \tag{8.21}$$

From (8.21) we see that the thermal correction depends entirely upon the sign of λ_T/θ^*, since we have been operating under the assumption that α_2 is a small but finite quantity. Since $\theta^* > 0$ it follows that (8.21) shows that it is the latent heat λ_T which determines how the admissible region changes in a *global* fashion near the boundary $\Sigma = 0$. Namely if $\lambda_T > 0$, corresponding to a $2 \rightarrow 1$ transformation being exothermic, then the function $z > 0$ and globally the admissibility region expands beyond the curve $\Sigma = 0$. Similarly if $\lambda_T < 0$, an endothermic transformation, then the admissibility region contracts inward from the boundary $\Sigma = 0$.

Attention is now focused on the admissibility boundary $\acute{s} = 0$. The previous analysis for the boundary $\Sigma = 0$ is general up to (8.19), hence to determine how the boundary $\acute{s} = 0$ shifts we need to determine where $z > 0$ and $z < 0$ along $\acute{s} = 0$. Evaluating (8.19) along $\dot{s} = 0$ and inserting the result into (8.18) yields

$$\mathrm{sign}\,[z|_{\dot{s}=0}] = \mathrm{sign}\left[c^2 2\Delta\gamma\right] . \tag{8.22}$$

Recall that for our problem $\dot{s} > 0 \Rightarrow \Delta\gamma < 0$, thus (8.22) yields that $z < 0$ everywhere along $\dot{s} = 0$. Hence the admissibility region contracts inward from the boundary $\dot{s} = 0$.

9. Solutions Obeying a Thermal Version of the Kinetic Relation

9.1 Driving Traction

The driving traction was defined in the purely mechanical setting in (5.10). In the fully thermomechanical setting the driving traction $f(t)$ is defined by

$$f(t) = \tilde{f}(\gamma, \theta) \equiv [[\varepsilon]] - \langle\langle\tau\rangle\rangle[[\gamma]] - \langle\langle\theta\rangle\rangle[[\eta]] . \qquad (9.1)$$

Using the definition of the free energy, $\psi = \varepsilon - \theta\eta$, the jump in internal energy can be expressed

$$[[\varepsilon]] = [[\psi]] + \langle\langle\theta\rangle\rangle[[\eta]] + \langle\langle\eta\rangle\rangle[[\theta]] ,$$

where the jump in the product $\theta\eta$ has been expressed

$$[[\theta\eta]] = \langle\langle\theta\rangle\rangle[[\eta]] + \langle\langle\eta\rangle\rangle[[\theta]].$$

Substituting from these results into (9.1) produces the driving traction in the more useful form

$$f(t) = [[\psi]] - \langle\langle\tau\rangle\rangle[[\gamma]] + \langle\langle\eta\rangle\rangle[[\theta]] . \qquad (9.2)$$

The driving traction (9.2) is not what is commonly seen in the literature, the conventional definition of the driving traction (Abeyaratne and Knowles 1990b, Fried 1992) in terms of the free energy and stress is

$$f(t) = [[\psi]] - \langle\langle\tau\rangle\rangle [[\gamma]] . \tag{9.3}$$

The difference between these driving tractions arises from assumptions on the temperature fields. Form (9.3) assumes that the temperature fields are smooth, analogous to the displacement field. This smoothness implies that across all interfaces the jump in temperature vanish, including across any phase boundary. The form of the driving traction defined in this document (9.2) was proposed to account for a temperature field with a discontinuous nature. Note that (9.2) reduces to the form (9.3) if $[[\theta]] = 0$. It is also recognized that for isothermal problems, and thus all purely mechanical problems, that the correct form of the driving traction is given by (9.3). However, (9.3) is not necessarily correct for those problems with a separable energy, which allows for such temperature jumps.

A useful form of the driving traction may be obtained upon writing the first term on the right hand side of (9.2) as

$$[[\psi]] = \psi^{+} - \psi^{-} = \int_{\psi^{-}}^{\psi^{+}} d\psi . \tag{9.4}$$

By invoking the fundamental definitions for stress and entropy the free energy differential $d\psi$ can be expressed

$$d\psi = \frac{\partial\psi}{\partial\gamma}d\gamma + \frac{\partial\psi}{\partial\theta}d\theta = \tau d\gamma - \eta d\theta, \tag{9.5}$$

and thus the jump in free energy may be written

$$[[\psi]] = \int_{\gamma^-}^{\gamma^+}\tau d\gamma - \int_{\theta^-}^{\theta^+}\eta d\theta. \tag{9.6}$$

which allows the driving traction (9.2) to be written

$$f(t) = \int_{\gamma^-}^{\gamma^+}\tau d\gamma - \langle\langle\tau\rangle\rangle[[\gamma]] - \left(\int_{\theta^-}^{\theta^+}\eta d\theta - \langle\langle\eta\rangle\rangle[[\theta]]\right). \tag{9.7}$$

Once again for smooth temperature fields the term inside the brackets vanishes, retrieving the more commonly used definition of the driving traction (9.3).

In Chapter 5 the driving traction (5.10) for the purely mechanical problem was defined

$$f(t)^{\text{mech}} = \int\hat{\tau}(\gamma)\,d\gamma - \langle\langle\hat{\tau}(\gamma)\rangle\rangle[[\gamma]].$$

To understand relationship between the purely mechanical form (5.10) of the driving traction and the thermal/separable energy form (9.2), some consideration of the temperature field within the body is required. In a purely mechanical setting the temperature is of no consideration, it is assumed that the problem is isothermal. Furthermore, in hyperelasticity the stress is assumed to be derivable from a potential function, the strain energy function, here denoted $W(\gamma)$, and thus $\tau(\gamma) = \frac{\partial}{\partial\gamma}W(\gamma)$. Recall in working with the Helmholtz free energy that the stress is $\tau(\gamma, \theta) = \frac{\partial}{\partial\gamma}\psi(\gamma, \theta)$. Thus if the free energy does not depend on temperature (as in the purely mechanical case), then the Helmholtz free energy is equivalent to the strain energy function. Working under the assumption of hyperelasticity, the integral term of the driving traction (5.10) is

$$\int_{\gamma_1}^{\gamma_2}\tau(\gamma)\,d\gamma = \int_{\gamma_1}^{\gamma_2}\frac{\partial}{\partial\gamma}W(\gamma)\,d\gamma = [[W]],$$

the driving traction (5.10) is

$$f(t)^{\text{mech}} = [[W]] - \langle\langle\hat{\tau}(\gamma)\rangle\rangle[[\gamma]]\,. \tag{9.8}$$

Thus the definition of the driving traction (9.2) reduces to the proper form in the limit of the purely mechanical case (9.8). Comparing (9.7) with definition (9.8) for the special case of isothermal motions recovers the familiar form of the driving traction commonly prescribed for those problems which are purely mechanical in nature

$$f(t)\,\big|_{\text{isothermal motions}} = \int_{\gamma^-}^{\gamma^+}\tau\,d\gamma - \langle\langle\tau\rangle\rangle[[\gamma]] \equiv f(t)^{\text{mech}}\,. \tag{9.9}$$

Returning to definition (9.1) the local balance law $(2.7)_3$ permits the driving traction to be expressed in its simplest form

$$f(t) = -\langle\langle\theta\rangle\rangle[[\eta]], \tag{9.10}$$

which is the form of the driving traction which we choose to use in the rest of this document. Since $\langle\langle\theta\rangle\rangle > 0$, the second law restriction (8.5) can be written

$$f(t) \geq 0. \tag{9.11}$$

Therefore, we conclude that the second law of thermodynamics states that the driving traction acting on the interface must be positive. Writing out the driving traction for initial interaction via (9.10) gives

$$f = -\frac{1}{2}\left(\theta_T + \theta_{S^\circ}\right)\left(\eta_T - \eta_{S^\circ}\right), \tag{9.12}$$

or since $\eta_T = \eta_2$,

$$f = -\frac{1}{2}\left(\theta_T + \theta_{S^\circ}\right)\left(\eta_2 - \eta_{S^\circ}\right). \tag{9.13}$$

Since all field quantities can be decomposed into two parts via (3.92)-(3.94), the first bracketed quantity in (9.13) may be written

$$\theta_T + \theta_{S^\circ} = \theta_T^o + \theta_T^{\alpha_2} + \theta_{S^\circ}^o + \theta_{S^\circ}^{\alpha_2}. \tag{9.14}$$

The jump in entropy using (8.4) and (8.5) is

$$\eta_2 - \eta_{S^\circ} =$$

$$\rho C_{\gamma 2} \ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \rho c_2^2 \alpha_2 (\gamma_2 - \gamma^*) + \frac{\rho \lambda_T}{\theta^*} - \rho C_{\gamma 1} \ln\left(\frac{\theta_{S^\circ}^o + \theta_{S^\circ}^{\alpha_2}}{\hat{\theta}}\right) - \rho C_{\gamma 1} \ln\left(\frac{\hat{\theta}}{\theta^*}\right). \tag{9.15}$$

From this jump in entropy we foresee one of the major problems of this research topic, the driving traction has field variables, which are themselves complex functions, in a logarithmic fashion. To avoid this difficulty, we limit our attention to the OB equilibrium state.

9.2 Driving Traction for Separable Materials with OB Initial Conditions

We conclude our analysis of the driving traction by considering separable materials with OB initial states. Guided by the consideration of Chapter 8 it seems clear that consistency with the purely mechanical theory only occurs in the case of an omnibalanced initial state. In this case $(7.19)_1$ and (7.37) give that

$$\frac{-1}{2}\left(\theta_T + \theta_{S^\circ}\right) = -\left(\hat{\theta} + \frac{1}{2\dot{s}\rho C_{\gamma 1}} D^{\mathrm{mech}}(\Delta\gamma, \dot{s})\right) \qquad (\mathrm{OB}), \tag{9.16}$$

while (7.37), (8.4), (8.6) yield

$$\eta_2 - \eta_{S^{\circ}} = \rho C_{\gamma 2} \ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \frac{\rho \lambda_T}{\theta^*} - \rho C_{\gamma 1} \ln\left(\frac{\hat{\theta}}{\theta^*}\right) \tag{9.17}$$

$$-\rho C_{\gamma 1} \ln\left(1 + \frac{1}{\dot{s}\rho\hat{\theta}C_{\gamma 1}} D^{\mathrm{mech}}(\Delta\gamma, \dot{s})\right) \qquad (\mathrm{OB})\,.$$

Recall for $c_1 = c_2$ that omnibalanced states involve initial temperatures $\hat{\theta}$ obeying $(4.32)_1$ in the $\alpha_2 \to 0$ limit. In this case (9.17) further simplifies to

$$\eta_2 - \eta_{S^{\circ}} = -\rho C_{\gamma 1} \ln\left(1 + \frac{1}{\dot{s}\rho\hat{\theta}C_{\gamma 1}} D^{\mathrm{mech}}(\Delta\gamma, \dot{s})\right) \qquad (c_1 = c_2, \mathrm{OB})\,. \tag{9.18}$$

Thus for an omnibalanced initial state, the $\alpha_2 \to 0$ limit of the driving traction is given by

$$f^{\circ} = \rho C_{\gamma 1}\left(\hat{\theta} + \frac{D^{\mathrm{mech}}(\Delta\gamma, \dot{s})}{2\dot{s}\rho C_{\gamma 1}}\right) \ln\left(1 + \frac{D^{\mathrm{mech}}(\Delta\gamma, \dot{s})}{\dot{s}\rho C_{\gamma 1}\hat{\theta}}\right) \qquad (c_1 = c_2, \mathrm{OB})\,. \tag{9.19}$$

Recall that the omnibalanced temperature $(4.32)_1$ is

$$\hat{\theta}^{\mathrm{OBO}} = \theta^* \exp\left(\frac{\lambda_T}{\theta^*(C_{\gamma 1} - C_{\gamma 2})}\right).$$

Note if the latent heat is nonvanishing then the limit $C_{\gamma 1} \to C_{\gamma 2}$ gives that the temperature $\hat{\theta}^{\mathrm{OBO}} \to \infty$. This limit permits the logarithmic expression in (9.19) to be expanded via a Taylor series

$$\ln\left(1+\frac{D^{\mathrm{mech}}(\Delta\gamma,\dot{s})}{\dot{s}\rho C_{\gamma 1}\hat{\theta}}\right)=\frac{D^{\mathrm{mech}}(\Delta\gamma,\dot{s})}{\dot{s}\rho C_{\gamma 1}\hat{\theta}}+O\left(\hat{\theta}^{-2}\right). \tag{9.20}$$

Using result (9.20) simplifies (9.19)

$$f^{o}=\frac{C_{\gamma 1}\rho}{2}\left(2\hat{\theta}+\frac{D^{\mathrm{mech}}(\Delta\gamma,\dot{s})}{\dot{s}\rho C_{\gamma 1}}\right)\left(\frac{D^{\mathrm{mech}}(\Delta\gamma,\dot{s})}{\dot{s}\rho C_{\gamma 1}\hat{\theta}}+O\left(\hat{\theta}^{-2}\right)\right)\qquad(\mathrm{OB}),$$

collecting like powers of $\hat{\theta}$ gives

$$f^{o}=\frac{D^{\mathrm{mech}}(\Delta\gamma,\dot{s})}{\dot{s}}+O\left(\hat{\theta}^{-1}\right)\qquad(\mathrm{OB}). \tag{9.21}$$

Thus for the case where the specific heats are the same and the initial state is omnibalanced we find that the separable form of the driving traction is

$$f^{o}=\frac{D^{\mathrm{mech}}(\Delta\gamma,\dot{s})}{\dot{s}}\qquad(C_{\gamma 1}=C_{\gamma 2},\ (\mathrm{OB})). \tag{9.22}$$

Note that (9.22) is equivalent to the driving traction that was found for the purely mechanical problem (5.11). Again we have demonstrated the close correspondence between the purely mechanical and the separable theories.

9.3 Kinetic Relation for Separable Materials

We now wish to consider the use of a kinetic relation to single out a particular phase boundary speed for separable materials with OB initial conditions. In Chapter 5 the use of a linear kinetic relation was investigated, and from (5.20) it is natural to assume that the kinetic relation for the case of a separable material is

$$\dot{s} = \kappa f^{o}. \tag{9.23}$$

Driven by result (9.22), we examine (9.23) for the same conditions. First, we note that for these initial conditions the dissipation function is given by (5.16), then with a specified mobility κ and initial conditions, (9.22) and (9.23) give an implicit equation for $\dot{s}$

$$\Delta\gamma = \frac{\dot{s}}{\kappa\rho c^2 (\gamma_1 - \gamma_2)} + \frac{\dot{s} c (\gamma_1 - \gamma_2)}{2(c^2 - \dot{s}^2)} \qquad (\mathrm{OB}). \tag{9.24}$$

This is result (5.23) found for the purely mechanical case, which was to be expected. Therefore Figure 5.3 being a graph in the $(\Delta\gamma, \dot{s})$ -plane of the linear kinetic relation (5.23) also describes the linear kinetic relation for a separable material. This figure shows the curve (9.24) for different values of the mobility κ, from the figure it is seen that as the mobility decreases the phase boundary speed decreases.

9.4 Kinetic Relation for Fully Thermal Materials

We now wish to include thermal effects in the linear kinetic relation. This change might yield a different value for the phase boundary speed from that determined in the separable theory Just as the change in the admissibility region could be determined by examining first order α_2 effects in the 2nd law as discussed in section 8.3, we expect that the change in the phase boundary speed can be accomplished by a similar analysis of the driving traction.

The linear kinetic relation is

$$\dot{s} = \kappa(f^{o} + f^{\alpha_2}), \tag{9.25}$$

where in the $\alpha_2 \to 0$ limit we retrieve the separable case (9.23). Thus the term κf^{α_2} participates in the thermal correction to the separable phase boundary speed (9.23). For OB initial states we find the leading order thermal correction to the driving traction can be expressed

$$\begin{aligned} f^{\alpha_2} = {} & -\rho\left(\hat{\theta} + \frac{D}{2\dot{s}\rho C_{\gamma 1}}\right)\left(c_2^2\alpha_2(\gamma_2 - \gamma^*) + C_{\gamma 1}\ln\left(1 + \frac{\theta_{S^\circ}^{\alpha_2}}{\hat{\theta} + \frac{D}{\dot{s}\rho C_{\gamma 1}}}\right)\right) \\ & -\left(\frac{\theta_T^{\alpha_2} + \theta_{S^\circ}^{\alpha_2}}{2}\right)\left(C_{\gamma 2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \frac{\lambda_T}{\theta^*} - C_{\gamma 1}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) - C_{\gamma 1}\ln\left(1 + \frac{D}{\dot{s}\rho C_{\gamma 1}\hat{\theta}}\right)\right) + O(\alpha_2^2). \end{aligned} \tag{9.26}$$

Note in (9.26) that the mechanical field variable $\theta_{S^{\circ}}^{\alpha_2}$ and the dissipation function D, both complicated functions, appear in the a logarithmic manner. Thus to determine the global behavior of f^{α_2} a numerical study might be in order. Since such an approach is not in the same vein as the rest of this investigation, a detailed analysis of f^{α_2} remains to be explored.

10. Conclusions and Recommendations for Future Work

10.1 Conclusions

From our analysis we have shown a number of results for the problem considered, most of these demonstrated how the purely mechanical theory falls under a more complete thermomechanical framework. Some of the more significant results are listed below.

1. For the mechanical field quantities of strain and velocity, a one to one correspondence exists between the purely mechanical and separable theories.

2. The positive dissipation criterion for the purely mechanical theory is a direct consequence of the second law of thermodynamics for the separable theory provided that the initial configuration is omnibalanced. Thus, the purely mechanical criterion has a sound thermodynamic foundation.

3. For a phase transformation occurring in a separable material, our model predicts the possibility for a temperature change within the transformed material. If the initial configuration is omnibalanced, then this change correlates directly with the dissipation function in the separable theory limit.

4. The separable theory, a theory which was shown to account for temperature effects, does not remove the nonuniqueness present in problems concerned with phase boundary motion. Thus, a higher order theory is required to resolve this issue. A reasonable resolu-

tion involves a separate kinetic relation.

10.2 Recommendations for Future Work

As with most research problems, there are a number of issues which we choose not to address here, of these some of the more significant ones are listed below.

1. Investigation of the shock instead of the centered simple wave fan needs to be completed. This may provide a simplification in analysis.

2. For the case $\alpha_2 \ll 1$, a more complete analysis of the admissible solution region needs to be performed to determine how it changes in comparison to the solution region from the separable theory. This may prove untenable due to the presence of complex functions contained within logarithms expressions.

3. Although this was a purely analytic study, a numerical study of the transformed materials temperature θ_{s^o} might prove fruitful. The results of such a study could be directly incorporated into a study of the admissible solution region. Recall that the growth of this region depends solely on the temperature θ_{s^o}.

4. For the case $\alpha_2 \ll 1$, a study of the incorporation of thermal effects into the linear kinetic relation needs to be performed. The results of such a study would determine if the inclusion of thermal effects would cause the phase boundary speed to increase or decrease from the speed found for a separable material.

Appendicies

Appendix A. Algorithm for Reduction of Equations (6.5)-(6.13)

The algorithm outlined below expresses the eight field quantities v_S, γ_S, θ_S, v_{S°, γ_{S°, θ_{S°, v_T, γ_T as functions in terms of the initial conditions, temperature θ_T, and the phase boundary speed. From (7.3) the temperature in region S

$$\theta_S = \hat{\theta}. \tag{A.1}$$

For later use we use (6.7) and (6.8) to relate the velocity and strain in regions S and So

$$v_S = v_{S^\circ}, \tag{A.2}$$

$$\gamma_S = \gamma_{S^\circ}. \tag{A.3}$$

From (6.9) the strain γ_T is found to be

$$\gamma_T = \gamma_2 + \frac{C_{\gamma 2}}{c_2^2 \alpha_2} \ln\left(\frac{\hat{\theta}}{\theta_T}\right), \tag{A.4}$$

while from (6.10) the velocity v_T is

$$v_T = \sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right], \tag{A.5}$$

where $\vartheta(\theta) = 2\Phi(\theta) + \Phi(0)\ln\left(\frac{\Phi(\theta) - \Phi(0)}{\Phi(\theta) + \Phi(0)}\right)$.Using results (A.2) and (A.3) we may rewrite (6.5)

$$v_{S^\circ} = c_1\gamma_{S^\circ} - c_1(\gamma_1 + 2\Delta\gamma)\,. \tag{A.6}$$

From (6.11) the velocity v_{S°

$$v_{S^\circ} = v_T + \dot{s}\,(\gamma_T - \gamma_{S^\circ})\,, \tag{A.7}$$

and from results (A.4) and (A.5) the expression for the velocity

$$v_{S^\circ} = \sqrt{C_{\gamma 2}}\Big(\vartheta(\theta_T) - \vartheta(\hat{\theta})\Big) + \dot{s}\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right) - \dot{s}\gamma_{S^\circ}\,. \tag{A.8}$$

Combining results (A.6) and (A.8) to find expressions for both the velocity and the strain in region S^0 in terms of the unknown temperature θ_T one finds

$$v_{S^\circ} = \frac{c_1}{c_1 + \dot{s}}\left(\sqrt{C_{\gamma 2}}\Big(\vartheta(\theta_T) - \vartheta(\hat{\theta})\Big) + \dot{s}\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right) - \dot{s}\,(\gamma_1 + 2\Delta\gamma)\right), \tag{A.9}$$

$$\gamma_{S^\circ} = \frac{1}{c_1 + \dot{s}}\left(\sqrt{C_{\gamma 2}}\Big(\vartheta(\theta_T) - \vartheta(\hat{\theta})\Big) + \dot{s}\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right) + c_1(\gamma_1 + 2\Delta\gamma)\right). \tag{A.10}$$

To express the field variable θ_{S° in terms of the temperature θ_T, insert results (A.4), (A.10) into equation (6.13), and by simplifying one finds

$$\theta_{S^\circ} = T_1(\theta_T) + T_2(\theta_T) + [T_3(\theta_T) + T_4(\theta_T)]\,T_5(\theta_T)\,, \tag{A.11}$$

where we have used the auxiliary functions

$$T_1(\theta_T) \equiv \frac{1}{\rho C_{\gamma 1}}\left(\frac{\rho c_2^2}{2}\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right) - (\gamma^* - \alpha_2\theta^*)\right)^2 + \rho C_{\gamma 2}\theta_T + \hat{b}_2 - \hat{b}_1\right),$$

$$T_2(\theta_T) \equiv \frac{-c_1^2}{2C_{\gamma 1}(c_1 + \dot{s})^2}\left(\sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right] + c_1(\gamma_1 + 2\Delta\gamma) + \dot{s}\left[\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right]\right)^2,$$

$$T_3(\theta_T) \equiv \frac{\rho c_1^2}{(c_1 + \dot{s})}\left(\sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right] + c_1(\gamma_1 + 2\Delta\gamma) + \dot{s}\left[\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right]\right),$$

$$T_4(\theta_T) \equiv \rho c_2^2\left(\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right) - (\gamma^* - \alpha_2\theta^*)\right) - \rho c_2^2\alpha_2\theta_T,$$

$$T_5(\theta_T) \equiv \frac{1}{2\rho C_{\gamma 1}(c_1 + \dot{s})}\left(\sqrt{C_{\gamma 2}}\left[\vartheta(\theta_T) - \vartheta(\hat{\theta})\right] + c_1(\dot{s} + 2\Delta\gamma) - c_1\left[\gamma_2 + \frac{C_{\gamma 2}}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta_T}\right)\right]\right).$$

Finally the master equation for the temperature θ_T is found by inserting results (A.4), (A.5), (A.9), (A.10) into equation (7.9) and simplifying

$$\sqrt{C_{\gamma 2}}(c_1 - \dot{s})\,\vartheta(\theta_T) - \frac{C_{\gamma 2}(\dot{s}c_1 - c_2^2)}{c_2^2\alpha_2}\ln\left(\frac{\theta_T}{\theta^*}\right) + c_2^2\alpha_2\theta_T =$$
$$\sqrt{C_{\gamma 2}}(c_1 - \dot{s})\,\vartheta(\hat{\theta}) - \frac{C_{\gamma 2}(\dot{s}c_1 - c_2^2)}{c_2^2\alpha_2}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) + c_2^2\alpha_2\hat{\theta} + (\dot{s}c_1 - c_1^2)2\Delta\gamma + \dot{s}c_1(\gamma_1 - \gamma_2)\,. \tag{A.12}$$

Appendix B. Transition in phase-2 is a shock

As discussed in Chapter 6, the characteristic curves in the phase-2 material are not globally parallel as is the case in phase-1. Therefore transitions between different states can occur through two types of mechanisms, a centered simple wave fan and a shock. As the case of the centered simple wave fan was analyzed in detail in Chapter 6 we now turn our attention to the case where the transition is a shock. The purpose of this appendix is to formulate the necessary equations which mathematically describe the shock problem.

Recall that if the transition was a centered simple wave fan then the Riemann invariants imposed a set of conditions between the field variables on adjacent sides of the fan. For the case of a shock these conditions need not be satisfied, instead a new set of constraints, the Rankine-Hugoniot equations, now must be satisfied. Recall that these equations were the jump conditions (2.7) across the phase boundary. This is because the phase boundary and the shock are discontinuity surfaces.The Rankine-Hugoniot equations across the shock are:

$$
\begin{aligned}
&[[v]] + \dot{h}[[\gamma]] = 0, \\
&[[\tau]] + \dot{h}\rho[[v]] = 0, \\
&\dot{h}([[\varepsilon]] - \langle\langle\tau\rangle\rangle[[\gamma]]) = 0, \\
&\dot{h}\rho[[\eta]] \le 0.
\end{aligned}
\tag{B.1}
$$

where $\dot{h}$ is the speed of the shock, which we assume to be constant, in view of the self-similar nature of the square-wave pulse that initiates the process.

We wish to reconsider a boundary value problem outlined in Chapter 6, except now where the T/E_2 interface is a shock, all other assumptions are assumed the same as the case of the centered simple wave fan. Thus, the dynamic boundary conditions (4.33)-(4.37) and assumptions A.5-A.9 (Chapter 5) still hold. These conditions give rise to an initial wave pulse, originating in the phase-1 material, striking the phase boundary and setting it in motion. Once again the pulse striking the phase boundary can generate a reflected wave, giving rise to regions R, S, S^o, and a transmitted wave, creating region T. However, now the T/E_2 interface is a shock, across which equations (B.1) are required to be satisfied.

Figure B.1 is a graphical representation in (xt)-space of the temporal changes within the body where the phase boundary speed is positive. During the initial encounter there are four regions of interaction which are of interest, these four have been labeled R,S,S^o and T in Figure B.1. One can think of these regions as follows: S is the region to the left of the initial position of the phase boundary in which the initial pulse and the wave which has been reflected from the phase boundary are interacting; S^o is that region to the right of the initial position of the phase boundary in which the incoming pulse and the reflected wave are interacting, R is the result of initial incoming pulse being reflected from the phase boundary and clear of any further interactions, finally the region T is that region in which some part of the initial pulse has transmitted through the phase boundary. The shock is to occur between the phase-2 equilibrium state and the T region.

As was the case for the fan, region R, which contains the final reflected wave, occurs later than either S or S^o and thus decouples from the other three regions. Therefore, when analyzing the initial interaction we only need to consider the regions S, S^o, and T. We again use the method of characteristics to relate the various regions of the domain, between S and the incoming pulse-the Riemann invariants (3.51) and (3.52); between regions S and S^o-the two Riemann invariants (3.52), across the moving phase boundary between T and the S^o-the 3 jump conditions (2.7), between T and the initial phase-2 equilibrium state-the three shock conditions (B.1). In Figure B.1 the various characteristics and Riemann invariants are shown, as well as the jump conditions across the phase boundary, and the shock conditions in the phase-2 region.

From the procedure outlined above we generate ten equations between the nine field quantities: θ_S, θ_{So}, θ_T, γ_S, γ_{So}, γ_T, v_S, v_{So}, v_T, the shock speed $\dot{h}$, and the phase boundary speed $\dot{s}$. Guided by Figure B.1 and the above outline, the ten equations which govern the interactions between the S, S^o, and T are written out below.

Region S and the incoming pulse

$$v_S - c_1\gamma_s = -c_1(\gamma_1 + 2\Delta\gamma)\,, \tag{B.2}$$

$$\rho C_{\gamma 1}\ln\left(\frac{\theta_S}{\theta^*}\right) + \tilde{k}_1 = \rho C_{\gamma 1}\ln\left(\frac{\hat{\theta}}{\theta^*}\right) + \tilde{k}_1\,. \tag{B.3}$$

Region S and S_o

$$v_{S^o} - c_1\gamma_{S^o} = v_S - c_1\gamma_S\,, \tag{B.4}$$

$$v_{S^\circ} + c_1\gamma_{S^\circ} = v_S + c_1\gamma_S . \tag{B.5}$$

Region T and the phase-2 equilibrium state, characterized by the formation of the shock wave

$$-\dot{h}\,(\gamma_2 - \gamma_T) = v_2 - v_T , \tag{B.6}$$

$$\dot{h}\rho v_T = \rho c_2^2(\gamma_2 - \gamma^*) - \rho c_2^2\alpha_2(\hat{\theta} - \theta^*) - \rho c_2^2(\gamma_T - \gamma^*) + \rho c_2^2\alpha_2(\theta_T - \theta^*) , \tag{B.7}$$

$$\begin{gathered}\left[\frac{\rho c_2^2}{2}\left(\gamma_2 - \gamma^* + \alpha_2\theta^*\right)^2 + \rho C_{\gamma 2}\hat{\theta} + \hat{b}_2\right] - \left[\frac{\rho c_2^2}{2}\left(\gamma_T - \gamma^* + \alpha_2\theta^*\right)^2 + \rho C_{\gamma 2}\theta_T + \hat{b}_2\right] = \\ \frac{1}{2}\Big(\rho c_2^2(\gamma_2 - \gamma^*) - \rho c_2^2\alpha_2(\hat{\theta} - \theta^*) + \rho c_2^2(\gamma_T - \gamma^*) - \rho c_2^2\alpha_2(\theta_T - \theta^*)\Big)(\gamma_2 - \gamma_T) .\end{gathered} \tag{B.8}$$

Region S_0 and T

$$-\dot{s}\,(\gamma_T - \gamma_{S^\circ}) = v_T - v_{S^\circ} , \tag{B.9}$$

$$-\dot{s}\rho\,(v_T - v_{S^\circ}) = \rho c_2^2(\gamma_T - \gamma^*) - \rho c_2^2\alpha_2(\theta_T - \theta^*) - \rho c_1^2\gamma_{S^\circ} , \tag{B.10}$$

$$\begin{gathered}\left[\frac{\rho c_2^2}{2}\left(\gamma_T - \gamma^* + \alpha_2\theta^*\right)^2 + \rho C_{\gamma 2}\theta_T + \hat{b}_2\right] - \left[\frac{\rho c_1^2}{2}\gamma_{S^\circ}^2 + \rho C_{\gamma 1}\theta_{S^\circ} + \hat{b}_1\right] = \\ \frac{1}{2}\Big(\rho c_1^2\gamma_{S^\circ} + \rho c_2^2(\gamma_T - \gamma^*) - \rho c_2^2\alpha_2(\theta_T - \theta^*)\Big)(\gamma_T - \gamma_{S^\circ}) .\end{gathered} \tag{B.11}$$

The above equations are a system of ten equations for the eleven quantities γ_S, v_S, θ_S, γ_{S°, v_{S°, θ_{S°, γ_T, v_T, θ_T, $\dot{h}$, $\dot{s}$ this system of equations completely characterize the initial interaction.

Comparing this set, to that of (6.5)-(6.13) for a fan, it is to be noted that we have obtained an extra unknown $\acute{h}$, and an extra equation. The extra equation is due to the fact that 3 shock conditions are given across a T/E_2 shock interface, whereas only 2 characteristic equations held across a T/E_2 fan. On the other hand, the equations obtained here, (B.9)-(B.11), are simpler than those which describe the fan, (6.9) and (6.10), because those for the shock have no unknown field quantities appearing in a logarithmic fashion.

Preliminary studies indicate that an elimination procedure similar to that employed in Chapter 6 yields a master equation which would be the analogue of (6.14). This master equation is in terms of the strain γ_T, and is given by the following equation:

$$\rho\left(\frac{-c_2}{\dot{s}+c_1}(\gamma_T-(\gamma^*-\alpha_2\theta^*))+\frac{\dot{s}c_1}{\dot{s}+c_1}\gamma_T-c_1(\gamma_1+2\Delta\gamma)+\right.$$

$$\frac{c_2^2\alpha_2}{(\dot{s}-c_1)}\frac{\rho c_2^2\left[(\gamma_T-(\gamma^*-\alpha_2\theta^*))^2-(\gamma_2-(\gamma^*-\alpha_2\theta^*))^2\right]-2\rho C_{\gamma 2}\hat{\theta}}{(\rho c_2^2\alpha_2(\gamma_2-\gamma_T)-2\rho C_{\gamma 2})}+$$

$$\left.\frac{c_2^2\alpha_2}{(\dot{s}-c_1)}\frac{\left[\rho c_2^2(\gamma_T-(\gamma^*-\alpha_2\theta^*))+\rho c_2^2(\gamma_2-(\gamma^*-\alpha_2\theta^*))-\rho c_2^2\alpha_2\hat{\theta}\right](\gamma_2-\gamma_T)}{(\rho c_2^2\alpha_2(\gamma_2-\gamma_T)-2\rho C_{\gamma 2})}\right)^2$$

$$-\left[\rho c_2^2(\gamma_2-(\gamma^*-\alpha_2\theta^*))-\rho c_2^2\alpha_2\hat{\theta}-\rho c_2^2(\gamma_T-(\gamma^*-\alpha_2\theta^*))\right](\gamma_2-\gamma_T)+$$

$$\rho c_2^2\alpha_2(\gamma_2-\gamma_T)\left(\frac{\left[\rho c_2^2(\gamma_T-(\gamma^*-\alpha_2\theta^*))+\rho c_2^2(\gamma_2-(\gamma^*-\alpha_2\theta^*))-\rho c_2^2\alpha_2\hat{\theta}\right](\gamma_2-\gamma_T)}{(\rho c_2^2\alpha_2(\gamma_2-\gamma_T)-2\rho C_{\gamma 2})}\right.$$

$$\left.+\frac{\rho c_2^2\left[(\gamma_T-(\gamma^*-\alpha_2\theta^*))^2-(\gamma_T-(\gamma^*-\alpha_2\theta^*))^2\right]-2\rho C_{\gamma 2}\hat{\theta}}{(\rho c_2^2\alpha_2(\gamma_2-\gamma_T)-2\rho C_{\gamma 2})}\right)=0.$$

One would anticipate that this equation can be analyzed in a fashion similar to the case of a fan.

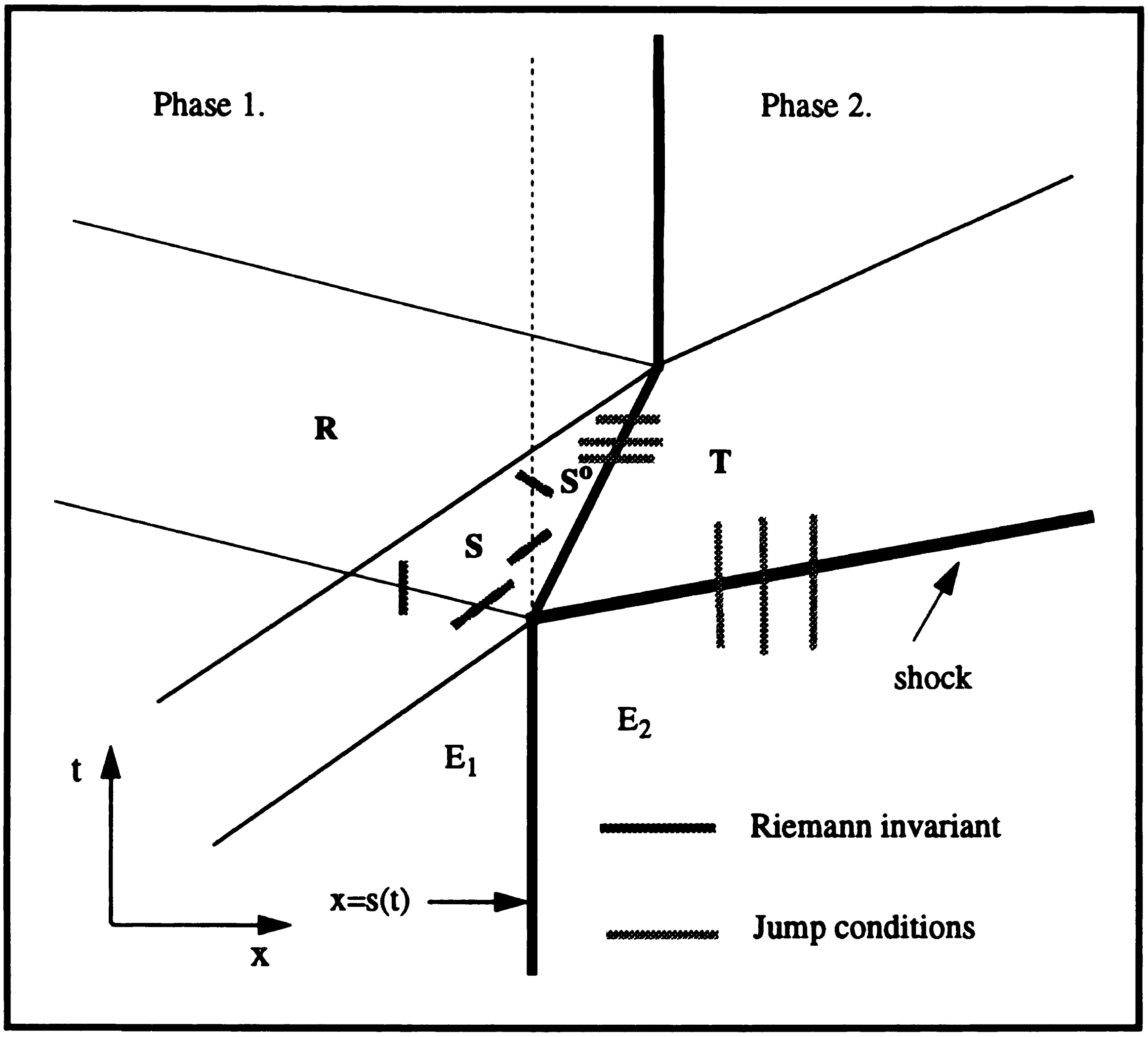

Figure B.1 This is a graphical representation in the (xt)-plane where the transition in the phase-2 regions gives rise the formation of a shock. Regions E_1 and E_2 are the initial equilibrium states separated by the phase boundary at x=s(t). The incoming wave (IW) strikes the phase boundary setting it into motion, where $\dot{s} > 0$ is assumed. The IW-phase boundary interaction gives rise to the regions S, S^o and R in phase-1, and T and the shock in phase-2. The region R represents a reflected wave, while S arises from the interaction of the IW and the reflected wave. S^o is that material which has undergone a phase transformation from phase-1 to phase-2. The IW striking the phase boundary also produces a transmitted wave in phase-2, this is designated by the letter T. Finally the transition from the E_2 state to the T state is a shock, and so involves 3 shock conditions, and the introduction of an yet unknown shock speed $\dot{h}$, whose value must be between c_{E_2} and c_T, where $c_T > c_{E_2}$. This figure, in conjunction with figure 6.1, give the two essential ways in which the purely mechanical situation displayed in Figure 5.1 are complicated by thermal effects in the adiabatic limit.

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